



## Full wwPDB EM Validation Report ⓘ

Jun 17, 2025 – 12:10 PM JST

PDB ID : 8YZI / pdb\_00008yzi  
EMDB ID : EMD-39694  
Title : The structure of PDCoV RBD and dog APN complex  
Authors : Sun, J.Q.; Niu, S.  
Deposited on : 2024-04-07  
Resolution : 3.05 Å(reported)

This is a Full wwPDB EM Validation 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 Phenix2.0rc1  
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

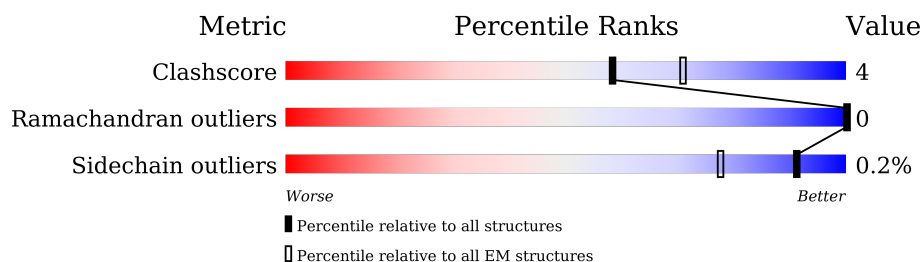
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.05 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  $\geq 3$ , 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	132	67% 20% 13%
1	C	132	69% 18% 13%
2	B	940	84% 12% .
2	D	940	86% 9% .
3	E	2	50% 50%
3	F	2	100%
3	H	2	100%
3	I	2	100%
3	J	2	50% 50%

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
3	K	2	 100%
3	L	2	 100%
3	M	2	 100%
3	N	2	 50%50%
4	G	2	 100%

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 16699 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 Spike protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	115	Total	C	N	O	S	0	0
			898	560	149	178	11		
1	A	115	Total	C	N	O	S	0	0
			898	560	149	178	11		

- Molecule 2 is a protein called Aminopeptidase N.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	900	Total	C	N	O	S	0	0
			7263	4654	1213	1373	23		
2	D	900	Total	C	N	O	S	0	0
			7263	4654	1213	1373	23		

- 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	E	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	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		

*Continued on next page...*

Continued from previous page...

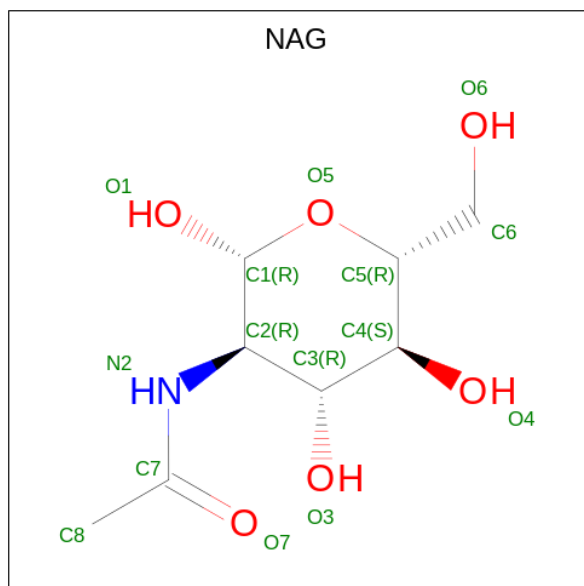
Mol	Chain	Residues	Atoms				AltConf	Trace
3	L	2	Total	C	N	O	0	0
			28	16	2	10		
3	M	2	Total	C	N	O	0	0
			28	16	2	10		
3	N	2	Total	C	N	O	0	0
			28	16	2	10		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
4	G	2	Total	C	N	O	0	0
			25	14	1	10		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

Continued on next page...

*Continued from previous page...*

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

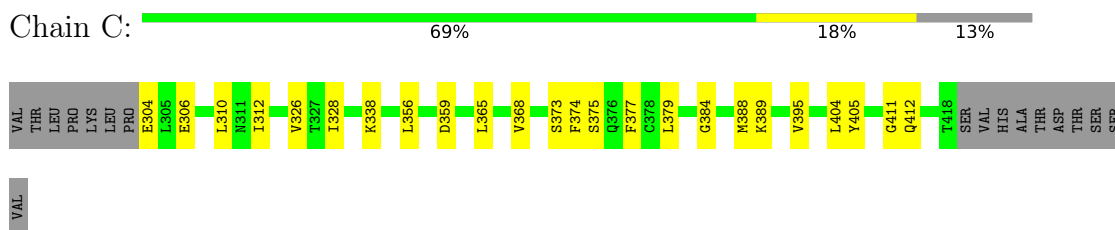
- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
6	B	1	Total	Zn	0
			1	1	
6	D	1	Total	Zn	0
			1	1	

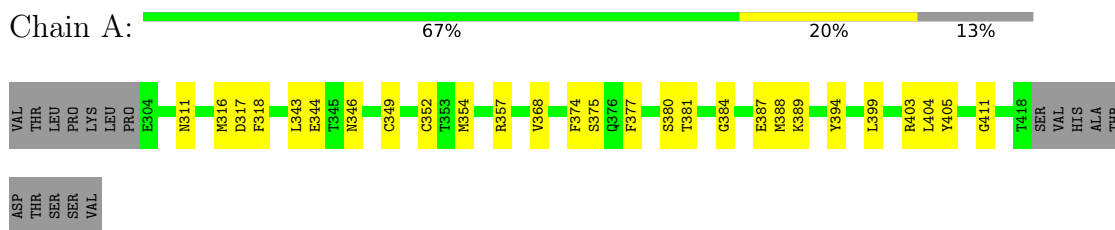
### 3 Residue-property plots

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.

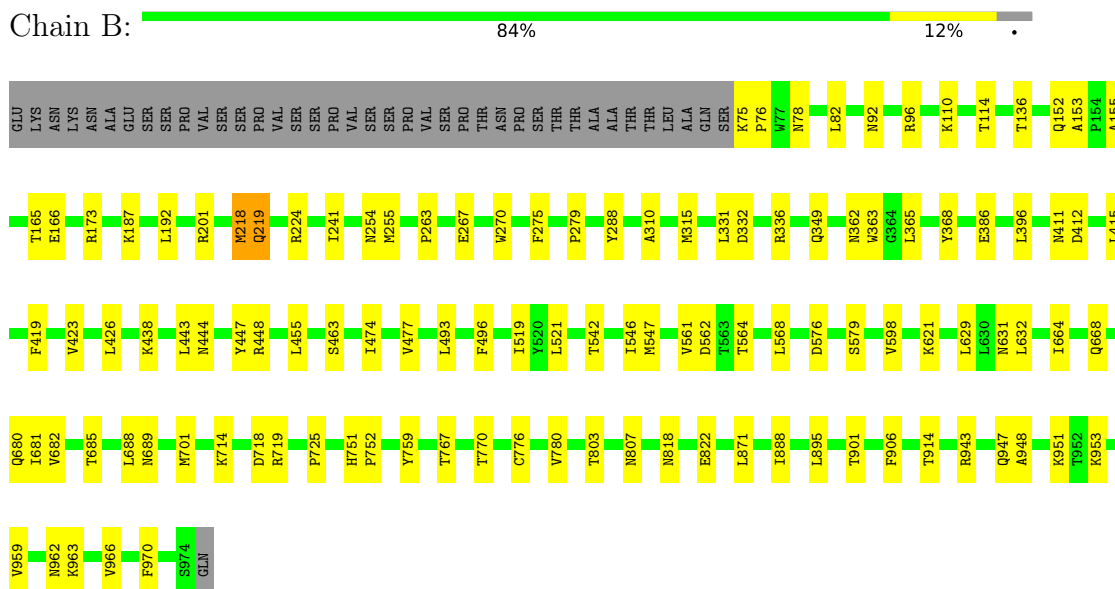
- Molecule 1: Spike protein



- Molecule 1: Spike protein



- Molecule 2: Aminopeptidase N



- Molecule 2: Aminopeptidase N

Y899	L493		R201		GLU
G900	S494				ASN
T901			Q219		LYS
F906	E499				ASN
	N500		D222		ALA
T910	L501				GLU
Q911			K225		SER
R915	N533		T238		SER
	Q534		F239		VAL
D935					SER
	V698		M255		SER
K951					PRO
N955	L632		T278		VAL
I956	N633				SER
K957	V634		T283		SER
			Y284		PRO
	T685		L285		VAL
W969					SER
F970	Y700		T300		SER
					PRO
S974	P725		V304		VAL
GLN					SER
	R731		I308		PRO
			W309		THR
	V734		A310		ASN
					PRO
	F738		M315		SER
					THR
	D750		R325		THR
					ALA
	T756		I330		ALA
					THR
	T767		Y342		THR
	A768		P343		LEU
	C769				ALA
	T770		Q349		ALA
					GLN
	K775		N356		SER
	C776				K75
	P798		M362		L82
	R801		L365		H129
	C806		Q378		I138
					Q139
			M403		
	T809				P154
			A431		
	E816		T470		E174
					P175
	V820		Q473		L176
			I474		
	A839		V477		Y182
	T856				L192
					D195
	1862		R491		L196
			W492		

- NAG1  
NAG2

- NAG1  
NAG2

- NAG1  
NAG2

- NAG1  
NAG2

- Chain J:  50% 50%





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

Chain K:  100%



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

Chain L:  100%



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

Chain M:  100%



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

Chain N:  50% 50%



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

Chain G:  100%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	90772	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	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, ZN

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	0.09	0/913	0.26	0/1238
1	C	0.08	0/913	0.29	1/1238 (0.1%)
2	B	0.13	0/7457	0.34	1/10172 (0.0%)
2	D	0.13	0/7457	0.33	1/10172 (0.0%)
All	All	0.13	0/16740	0.33	3/22820 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	219	GLN	N-CA-C	7.71	119.32	111.07
1	C	395	VAL	N-CA-C	-6.21	106.91	112.12
2	D	219	GLN	N-CA-C	6.12	117.62	111.07

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	898	0	859	18	0
1	C	898	0	859	14	0
2	B	7263	0	7059	70	0
2	D	7263	0	7060	49	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	28	0	25	0	0
3	F	28	0	25	0	0
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
3	L	28	0	25	0	0
3	M	28	0	25	0	0
3	N	28	0	25	1	0
4	G	25	0	22	0	0
5	A	14	0	13	0	0
5	B	42	0	39	1	0
5	C	14	0	13	0	0
5	D	28	0	26	0	0
6	B	1	0	0	0	0
6	D	1	0	0	0	0
All	All	16699	0	16175	147	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.

All (147) 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:343:LEU:HD12	1:A:368:VAL:HG11	1.68	0.74
1:C:306:GLU:HB2	1:C:338:LYS:HD2	1.74	0.69
2:B:255:MET:HE1	2:B:279:PRO:HD2	1.75	0.69
2:D:330:ILE:HD11	2:D:431:ALA:HB2	1.75	0.69
2:B:411:ASN:ND2	2:B:463:SER:O	2.23	0.69
1:C:359:ASP:HB2	1:C:389:LYS:HG3	1.74	0.68
1:C:359:ASP:OD1	1:C:389:LYS:NZ	2.25	0.67
2:D:491:ARG:NH2	2:D:634:VAL:O	2.28	0.67
2:D:310:ALA:HB3	2:D:315:MET:HE3	1.79	0.65
2:D:598:VAL:HG23	2:D:632:LEU:HD11	1.79	0.64
2:B:423:VAL:HG13	2:B:426:LEU:HD12	1.80	0.64
2:B:803:THR:O	2:B:807:ASN:ND2	2.31	0.64
2:D:195:ASP:OD2	2:D:225:LYS:NZ	2.31	0.63
1:A:317:ASP:OD1	2:D:325:ARG:NH1	2.31	0.63
2:B:241:ILE:HG12	2:B:288:TYR:HE1	1.65	0.61
1:A:344:GLU:OE1	1:A:346:ASN:ND2	2.34	0.61
1:C:375:SER:HB3	1:C:411:GLY:HA3	1.83	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:349:GLN:HG3	2:B:368:TYR:HE1	1.67	0.60
2:D:798:PRO:HA	2:D:801:ARG:HG3	1.83	0.60
2:B:455:LEU:HD22	2:B:947:GLN:NE2	2.16	0.59
2:B:631:ASN:HB3	2:B:668:GLN:HE22	1.67	0.59
2:B:959:VAL:O	2:B:963:LYS:HG3	2.02	0.59
1:A:387:GLU:OE2	1:A:403:ARG:NH1	2.36	0.58
2:B:493:LEU:HB2	2:B:547:MET:HE3	1.86	0.58
2:B:564:THR:O	2:B:621:LYS:NZ	2.37	0.58
2:D:767:THR:HA	2:D:770:THR:HG22	1.86	0.57
2:B:331:LEU:HD21	2:B:396:LEU:HD22	1.87	0.57
2:D:533:ASN:HB3	3:N:1:NAG:O5	2.04	0.57
2:B:96:ARG:HH21	2:B:110:LYS:HD2	1.70	0.56
1:C:304:GLU:HG3	1:C:338:LYS:HD3	1.87	0.56
1:A:394:TYR:HE2	2:D:378:GLN:HE22	1.52	0.56
2:B:75:LYS:NZ	2:B:78:ASN:OD1	2.38	0.56
1:A:311:ASN:OD1	1:A:346:ASN:ND2	2.37	0.56
2:D:700:TYR:HB3	2:D:756:THR:HG23	1.87	0.56
2:B:780:VAL:HG11	2:B:807:ASN:HB2	1.87	0.55
2:B:818:ASN:O	2:B:822:GLU:HG2	2.06	0.55
2:D:806:CYS:HB3	2:D:839:ALA:HA	1.88	0.55
2:D:951:LYS:HG3	2:D:955:ASN:HD21	1.72	0.55
2:D:470:THR:HG23	2:D:473:GLN:H	1.72	0.54
1:A:318:PHE:HE2	2:D:325:ARG:HD2	1.72	0.54
1:A:375:SER:HB3	1:A:411:GLY:HA3	1.90	0.54
2:B:562:ASP:OD2	2:B:564:THR:OG1	2.25	0.54
2:B:576:ASP:HB3	2:B:579:SER:HB3	1.90	0.54
2:B:192:LEU:HG	2:B:201:ARG:HB3	1.90	0.53
1:A:349:CYS:HB2	1:A:354:MET:HE3	1.91	0.53
2:B:386:GLU:OE1	2:B:759:TYR:OH	2.25	0.53
1:C:356:LEU:HD21	1:C:388:MET:HE2	1.91	0.52
2:B:263:PRO:HD3	5:B:1002:NAG:H62	1.92	0.51
2:B:680:GLN:HE22	2:B:962:ASN:HD21	1.59	0.51
2:D:856:THR:HA	2:D:862:ILE:HD11	1.91	0.51
1:A:388:MET:HB2	1:A:404:LEU:HB3	1.93	0.51
2:B:962:ASN:O	2:B:966:VAL:HG23	2.10	0.50
2:D:239:PHE:HZ	2:D:283:THR:HG22	1.76	0.50
2:B:914:THR:HG21	2:B:948:ALA:HB1	1.92	0.50
2:D:82:LEU:HD11	2:D:129:HIS:CE1	2.46	0.50
2:D:308:ILE:HD13	2:D:349:GLN:HB2	1.93	0.50
2:D:806:CYS:HA	2:D:809:ILE:HB	1.94	0.49
1:A:349:CYS:SG	1:A:352:CYS:HB2	2.52	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:255:MET:HE1	2:B:279:PRO:CD	2.41	0.49
2:B:166:GLU:OE2	2:B:224:ARG:NH1	2.45	0.49
1:C:365:LEU:HA	1:C:368:VAL:HG23	1.94	0.49
2:D:154:PRO:HB3	2:D:174:GLU:HB2	1.94	0.49
2:D:738:PHE:HE2	2:D:775:LYS:HE3	1.78	0.48
2:D:899:TYR:O	2:D:901:THR:N	2.46	0.48
2:D:176:LEU:HD22	2:D:182:TYR:CZ	2.49	0.48
2:B:455:LEU:HD21	2:B:951:LYS:HG2	1.94	0.48
2:B:871:LEU:HD13	2:B:888:ILE:HD11	1.96	0.47
2:D:196:LEU:HD13	2:D:356:ASN:HB3	1.96	0.47
1:C:384:GLY:HA3	1:C:405:TYR:HB3	1.96	0.47
2:B:92:ASN:HB3	2:B:114:THR:HB	1.96	0.47
2:B:426:LEU:HD23	2:B:438:LYS:HZ1	1.79	0.47
2:B:685:THR:O	2:B:689:ASN:HB2	2.13	0.47
1:A:357:ARG:NH2	2:D:750:ASP:OD2	2.46	0.47
1:A:380:SER:OG	1:A:381:THR:N	2.48	0.47
1:A:384:GLY:HA3	1:A:405:TYR:HB3	1.97	0.47
2:B:152:GLN:NE2	2:B:153:ALA:O	2.48	0.47
2:B:362:ASN:HB2	2:B:365:LEU:O	2.14	0.47
2:B:474:ILE:O	2:B:477:VAL:HG12	2.15	0.47
2:D:238:THR:OG1	2:D:278:THR:O	2.32	0.47
2:B:561:VAL:HG12	2:B:568:LEU:HB3	1.96	0.46
2:B:165:THR:O	2:B:165:THR:HG22	2.15	0.46
2:D:362:ASN:HB2	2:D:365:LEU:O	2.14	0.46
2:B:776:CYS:O	2:B:780:VAL:HG23	2.16	0.46
2:B:901:THR:O	2:B:901:THR:HG22	2.16	0.46
2:B:914:THR:HG22	2:B:914:THR:O	2.15	0.45
1:C:374:PHE:HB2	1:C:377:PHE:CE2	2.52	0.45
2:B:419:PHE:O	2:B:423:VAL:HG23	2.16	0.45
2:D:906:PHE:O	2:D:910:ILE:HG12	2.17	0.45
1:C:310:LEU:HD13	1:C:328:ILE:HG12	1.99	0.45
2:B:267:GLU:HB3	2:B:270:TRP:HD1	1.81	0.44
2:B:725:PRO:HB2	2:B:970:PHE:HB3	1.98	0.44
2:B:718:ASP:OD1	2:B:719:ARG:HG3	2.18	0.44
2:B:542:THR:O	2:B:546:ILE:HG13	2.17	0.44
2:D:816:GLU:O	2:D:820:VAL:HG22	2.18	0.44
2:D:138:ILE:HG22	2:D:139:GLN:N	2.32	0.44
2:D:300:THR:HG22	2:D:304:VAL:H	1.83	0.44
2:B:895:LEU:HB3	2:B:906:PHE:HZ	1.82	0.43
2:B:412:ASP:O	2:B:415:LEU:HD23	2.18	0.43
2:B:155:ALA:HB3	2:B:173:ARG:HE	1.82	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:731:ARG:HA	2:D:734:VAL:HG12	1.99	0.43
1:A:316:MET:HE3	1:A:316:MET:HB3	1.81	0.43
2:B:943:ARG:O	2:B:947:GLN:HG2	2.18	0.43
2:B:714:LYS:O	2:B:718:ASP:HB3	2.18	0.43
2:B:767:THR:HA	2:B:770:THR:HG22	2.00	0.43
2:D:494:SER:OG	2:D:499:GLU:OE1	2.37	0.43
2:D:911:GLN:O	2:D:915:ARG:HG3	2.17	0.43
1:C:404:LEU:HD23	1:C:404:LEU:H	1.84	0.43
2:B:267:GLU:HB3	2:B:270:TRP:CD1	2.53	0.42
2:D:769:CYS:N	2:D:776:CYS:SG	2.92	0.42
2:B:136:THR:HB	2:B:187:LYS:HG3	2.02	0.42
2:B:332:ASP:O	2:B:336:ARG:HG3	2.19	0.42
2:D:493:LEU:HD21	2:D:524:TRP:HZ3	1.83	0.42
2:D:285:LEU:HD13	2:D:403:ASN:HD22	1.84	0.42
2:B:241:ILE:HG23	2:B:275:PHE:HB2	2.02	0.42
2:D:255:MET:HE3	2:D:255:MET:HB3	1.90	0.42
1:A:389:LYS:HD2	1:A:399:LEU:HD11	2.01	0.42
1:C:312:ILE:HG13	1:C:326:VAL:HG13	2.01	0.42
2:B:664:ILE:HG12	2:B:701:MET:HE1	2.02	0.42
2:D:685:THR:HG23	2:D:969:TRP:CD1	2.55	0.42
2:D:935:ASP:N	2:D:935:ASP:OD1	2.53	0.42
1:A:374:PHE:HB2	1:A:377:PHE:CE2	2.55	0.42
2:B:82:LEU:H	2:B:82:LEU:HD23	1.85	0.41
2:D:956:ILE:HG13	2:D:957:LYS:H	1.85	0.41
2:D:501:LEU:HD21	2:D:534:GLN:HG2	2.01	0.41
2:B:493:LEU:HA	2:B:496:PHE:CE1	2.55	0.41
2:B:751:HIS:HA	2:B:752:PRO:HD3	1.92	0.41
2:B:310:ALA:HB3	2:B:315:MET:SD	2.61	0.41
2:B:953:LYS:H	2:B:953:LYS:HG2	1.71	0.41
1:A:316:MET:HG2	1:A:352:CYS:SG	2.61	0.41
2:D:342:TYR:HA	2:D:343:PRO:HD3	1.89	0.41
2:B:681:ILE:HG22	2:B:682:VAL:HG13	2.01	0.41
2:B:519:ILE:HD12	2:B:521:LEU:HD13	2.02	0.41
2:B:75:LYS:HA	2:B:76:PRO:HD3	1.88	0.41
2:B:444:ASN:O	2:B:448:ARG:NE	2.37	0.41
2:B:218:MET:HE2	2:B:218:MET:HB2	1.70	0.40
2:D:474:ILE:O	2:D:477:VAL:HG22	2.21	0.40
2:B:688:LEU:HD23	2:B:688:LEU:HA	1.93	0.40
2:D:725:PRO:HB2	2:D:970:PHE:HB3	2.04	0.40
2:D:951:LYS:HG3	2:D:955:ASN:ND2	2.35	0.40
1:C:379:LEU:HD11	1:C:404:LEU:HD12	2.03	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:598:VAL:HG13	2:B:632:LEU:HD11	2.03	0.40
2:B:629:LEU:HD12	2:B:629:LEU:HA	1.97	0.40
2:B:254:ASN:ND2	2:B:363:TRP:O	2.54	0.40
2:D:956:ILE:HG13	2:D:957:LYS:N	2.36	0.40
1:C:373:SER:HB3	1:C:412:GLN:HA	2.04	0.40
2:B:443:LEU:HD23	2:B:447:TYR:CD2	2.57	0.40
2:D:192:LEU:HG	2:D:201:ARG:HB3	2.04	0.40

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	113/132 (86%)	112 (99%)	1 (1%)	0	100	100
1	C	113/132 (86%)	110 (97%)	3 (3%)	0	100	100
2	B	898/940 (96%)	866 (96%)	32 (4%)	0	100	100
2	D	898/940 (96%)	868 (97%)	30 (3%)	0	100	100
All	All	2022/2144 (94%)	1956 (97%)	66 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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	103/119 (87%)	103 (100%)	0	100	100
1	C	103/119 (87%)	103 (100%)	0	100	100
2	B	803/839 (96%)	801 (100%)	2 (0%)	92	95
2	D	803/839 (96%)	802 (100%)	1 (0%)	92	96
All	All	1812/1916 (95%)	1809 (100%)	3 (0%)	91	95

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

Mol	Chain	Res	Type
2	B	218	MET
2	B	219	GLN
2	D	222	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	412	GLN
2	B	171	HIS
2	B	219	GLN
2	B	362	ASN
2	B	416	ASN
2	B	516	GLN
2	B	665	ASN
2	B	668	GLN
2	B	680	GLN
2	B	695	ASN
2	B	747	ASN
2	B	753	GLN
2	B	763	ASN
2	B	831	ASN
2	B	858	ASN
2	B	891	ASN
2	B	973	ASN
2	D	78	ASN
2	D	102	ASN
2	D	219	GLN
2	D	337	HIS
2	D	384	ASN
2	D	399	GLN
2	D	469	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	D	528	GLN
2	D	645	ASN
2	D	651	HIS
2	D	753	GLN
2	D	845	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 ⓘ

20 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	2,3	14,14,15	1.15	1 (7%)	17,19,21	1.00	1 (5%)
3	NAG	E	2	3	14,14,15	0.37	0	17,19,21	0.34	0
3	NAG	F	1	2,3	14,14,15	0.21	0	17,19,21	0.41	0
3	NAG	F	2	3	14,14,15	0.23	0	17,19,21	0.52	0
4	NAG	G	1	2,4	14,14,15	0.23	0	17,19,21	0.39	0
4	BMA	G	2	4	11,11,12	0.51	0	15,15,17	0.75	0
3	NAG	H	1	2,3	14,14,15	0.44	0	17,19,21	0.60	0
3	NAG	H	2	3	14,14,15	0.26	0	17,19,21	0.44	0
3	NAG	I	1	2,3	14,14,15	0.22	0	17,19,21	0.51	0
3	NAG	I	2	3	14,14,15	0.23	0	17,19,21	0.44	0
3	NAG	J	1	2,3	14,14,15	0.78	1 (7%)	17,19,21	0.78	1 (5%)
3	NAG	J	2	3	14,14,15	0.20	0	17,19,21	0.41	0
3	NAG	K	1	2,3	14,14,15	0.21	0	17,19,21	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	K	2	3	14,14,15	0.24	0	17,19,21	0.42	0
3	NAG	L	1	2,3	14,14,15	0.22	0	17,19,21	0.42	0
3	NAG	L	2	3	14,14,15	0.22	0	17,19,21	0.41	0
3	NAG	M	1	2,3	14,14,15	0.38	0	17,19,21	0.41	0
3	NAG	M	2	3	14,14,15	0.45	0	17,19,21	0.77	0
3	NAG	N	1	2,3	14,14,15	0.39	0	17,19,21	0.55	0
3	NAG	N	2	3	14,14,15	0.25	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
3	NAG	E	1	2,3	-	3/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1
3	NAG	F	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	3/6/23/26	0/1/1/1
4	NAG	G	1	2,4	-	2/6/23/26	0/1/1/1
4	BMA	G	2	4	-	0/2/19/22	0/1/1/1
3	NAG	H	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	H	2	3	-	0/6/23/26	0/1/1/1
3	NAG	I	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	I	2	3	-	0/6/23/26	0/1/1/1
3	NAG	J	1	2,3	-	4/6/23/26	0/1/1/1
3	NAG	J	2	3	-	0/6/23/26	0/1/1/1
3	NAG	K	1	2,3	-	0/6/23/26	0/1/1/1
3	NAG	K	2	3	-	2/6/23/26	0/1/1/1
3	NAG	L	1	2,3	-	0/6/23/26	0/1/1/1
3	NAG	L	2	3	-	0/6/23/26	0/1/1/1
3	NAG	M	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	M	2	3	-	4/6/23/26	0/1/1/1
3	NAG	N	1	2,3	-	0/6/23/26	0/1/1/1
3	NAG	N	2	3	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1	NAG	O5-C1	-4.12	1.37	1.43
3	J	1	NAG	O5-C1	-2.80	1.39	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1	NAG	C3-C4-C5	2.27	114.29	110.24
3	J	1	NAG	C3-C4-C5	2.12	114.02	110.24

There are no chirality outliers.

All (28) torsion outliers are listed below:

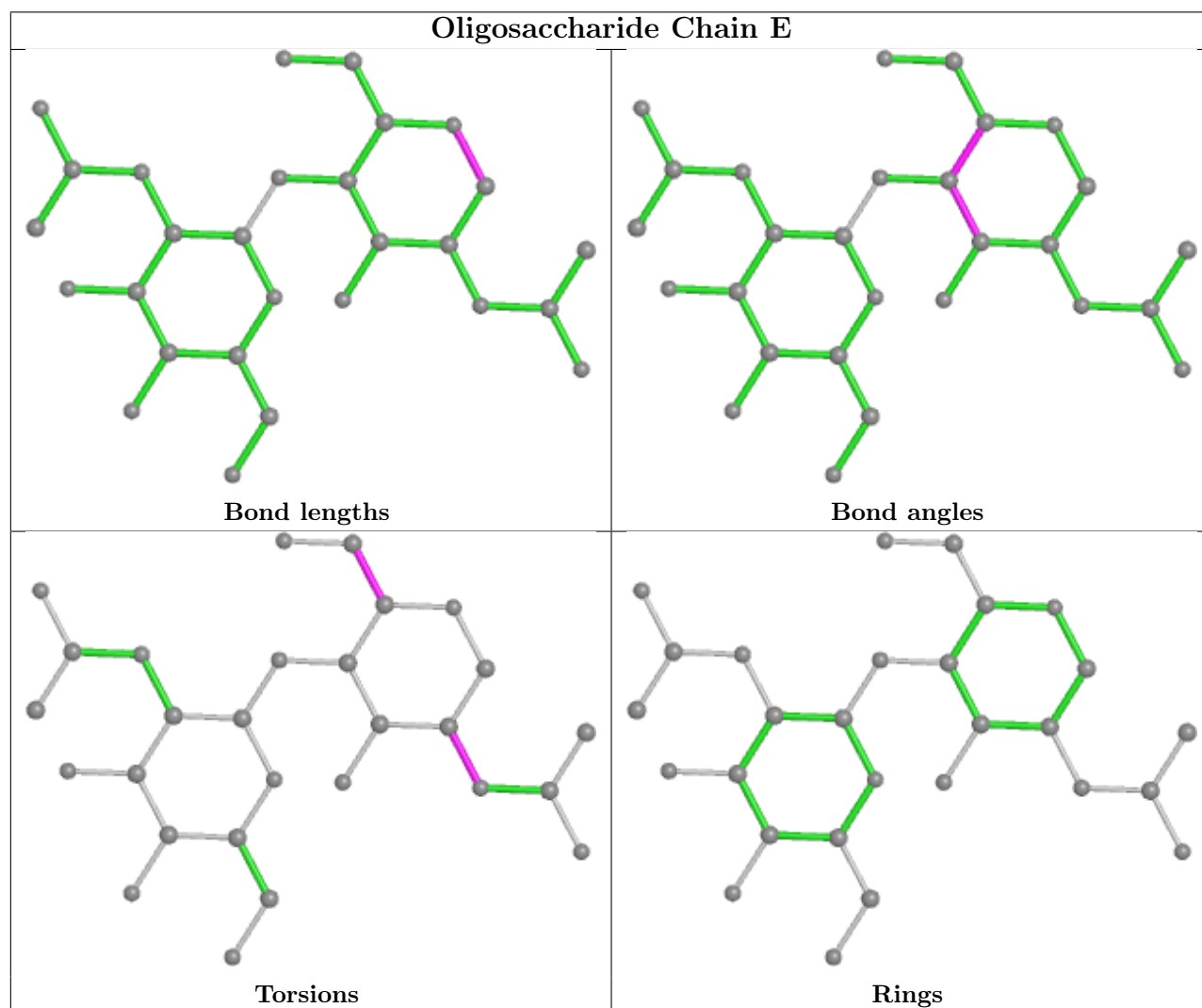
Mol	Chain	Res	Type	Atoms
3	I	1	NAG	C4-C5-C6-O6
3	M	2	NAG	O5-C5-C6-O6
3	H	1	NAG	C4-C5-C6-O6
3	H	1	NAG	O5-C5-C6-O6
3	I	1	NAG	O5-C5-C6-O6
3	M	2	NAG	C4-C5-C6-O6
3	J	1	NAG	C4-C5-C6-O6
3	N	2	NAG	C4-C5-C6-O6
3	F	1	NAG	C8-C7-N2-C2
3	F	1	NAG	O7-C7-N2-C2
3	J	1	NAG	C8-C7-N2-C2
3	J	1	NAG	O7-C7-N2-C2
4	G	1	NAG	C8-C7-N2-C2
4	G	1	NAG	O7-C7-N2-C2
3	K	2	NAG	O5-C5-C6-O6
3	K	2	NAG	C4-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
3	J	1	NAG	O5-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
3	N	2	NAG	O5-C5-C6-O6
3	M	1	NAG	C4-C5-C6-O6
3	M	1	NAG	O5-C5-C6-O6
3	E	1	NAG	C3-C2-N2-C7
3	F	2	NAG	C3-C2-N2-C7
3	E	1	NAG	O5-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
3	M	2	NAG	C3-C2-N2-C7
3	M	2	NAG	C1-C2-N2-C7

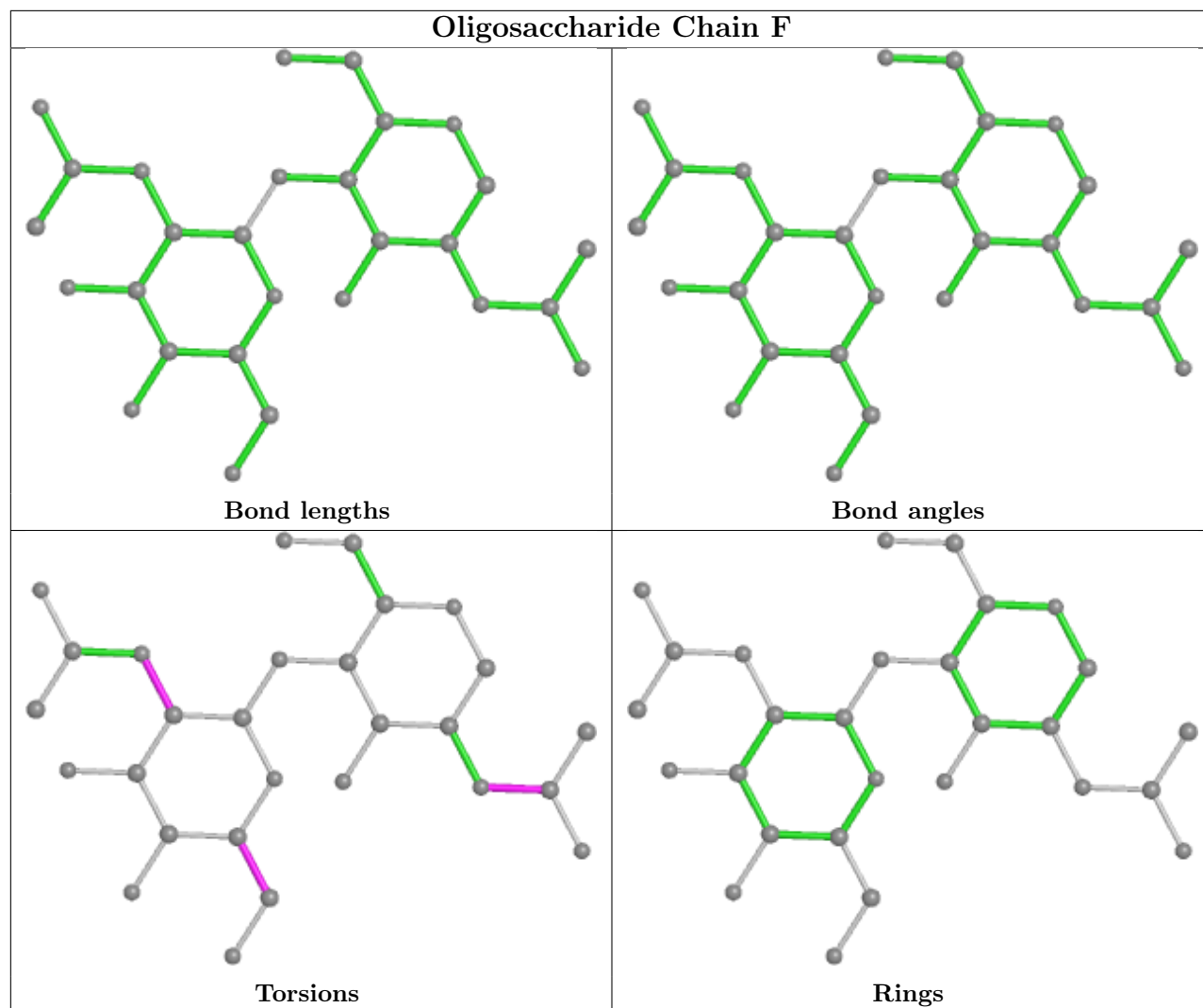
There are no ring outliers.

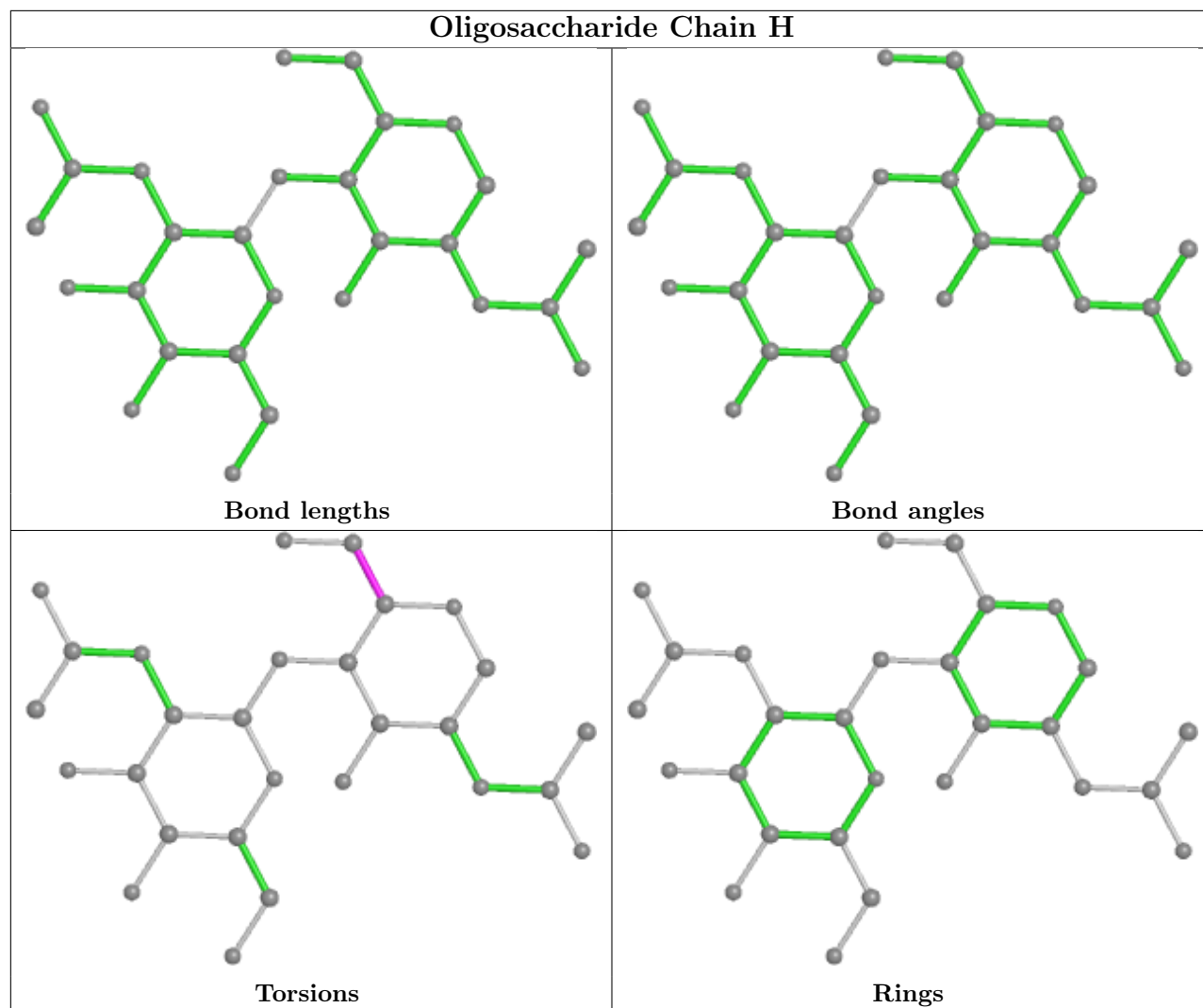
1 monomer is involved in 1 short contact:

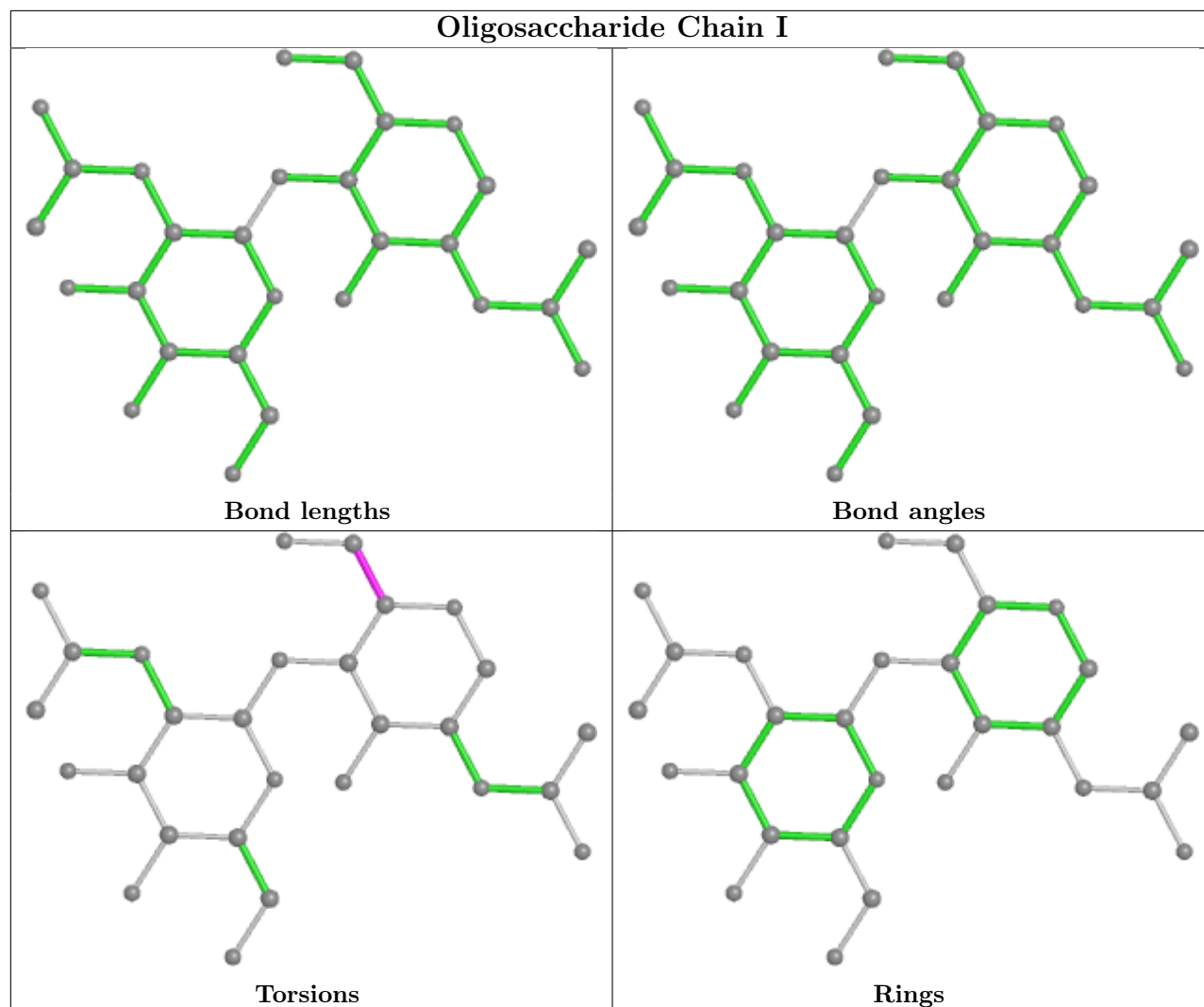
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	N	1	NAG	1	0

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

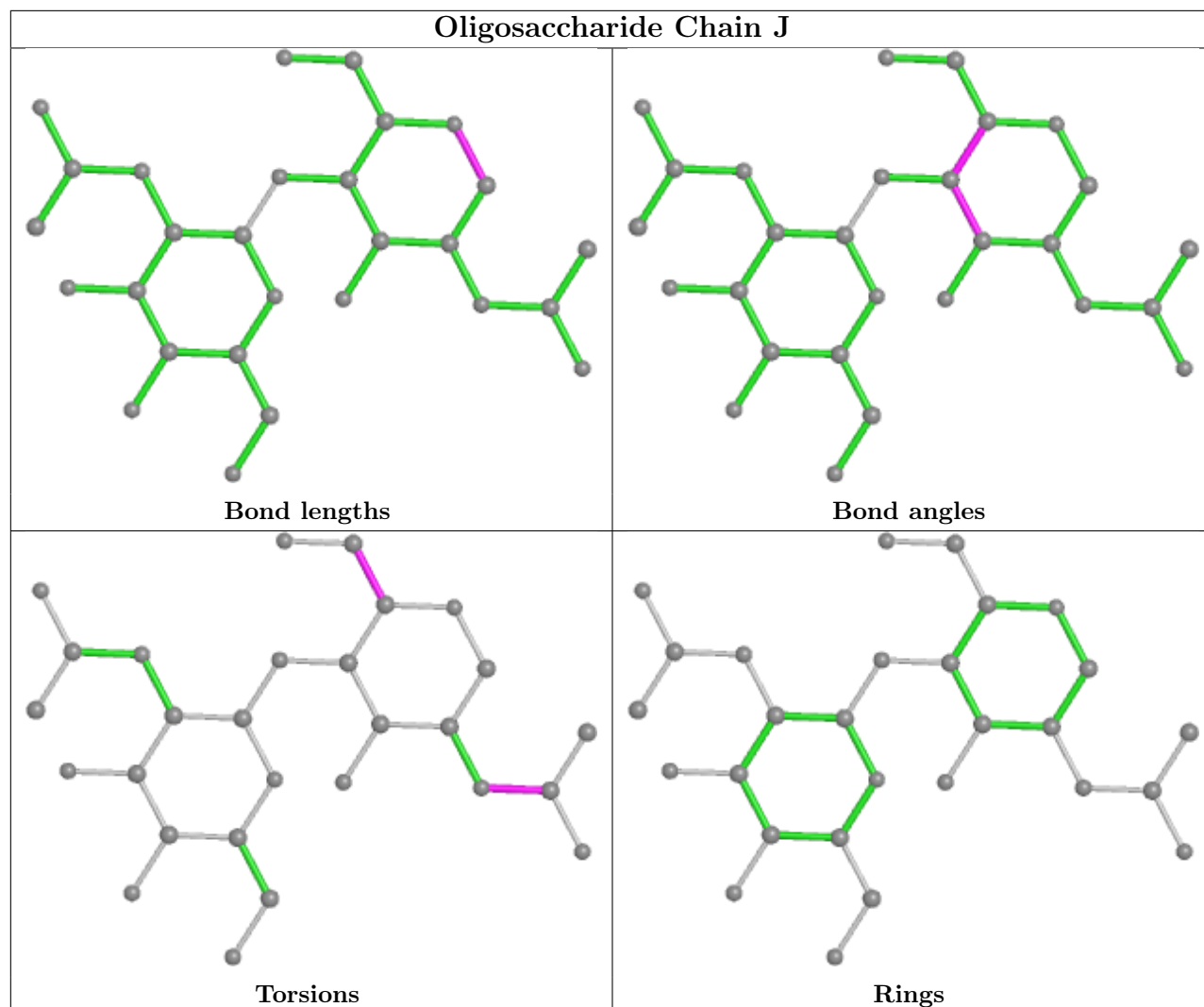


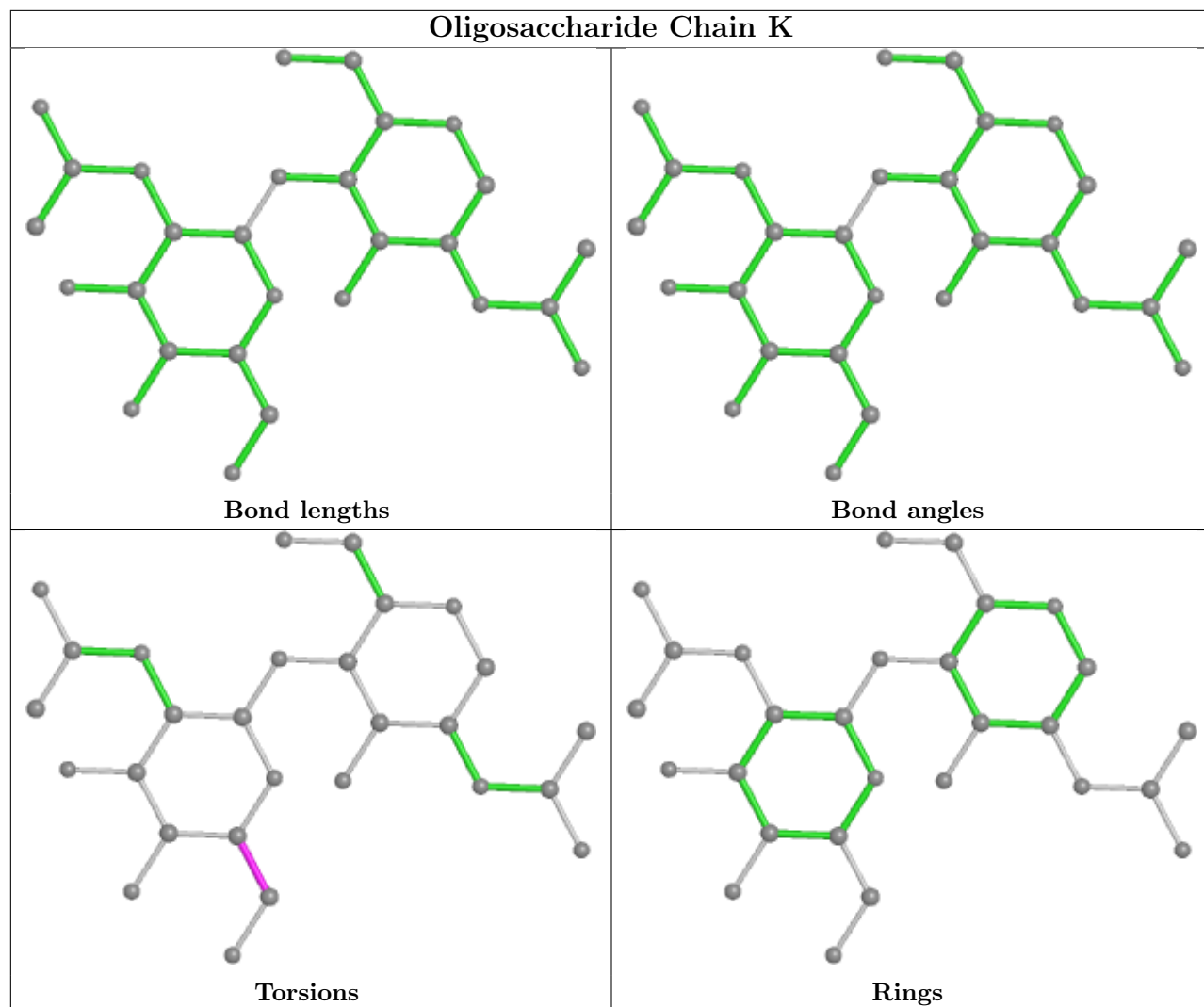


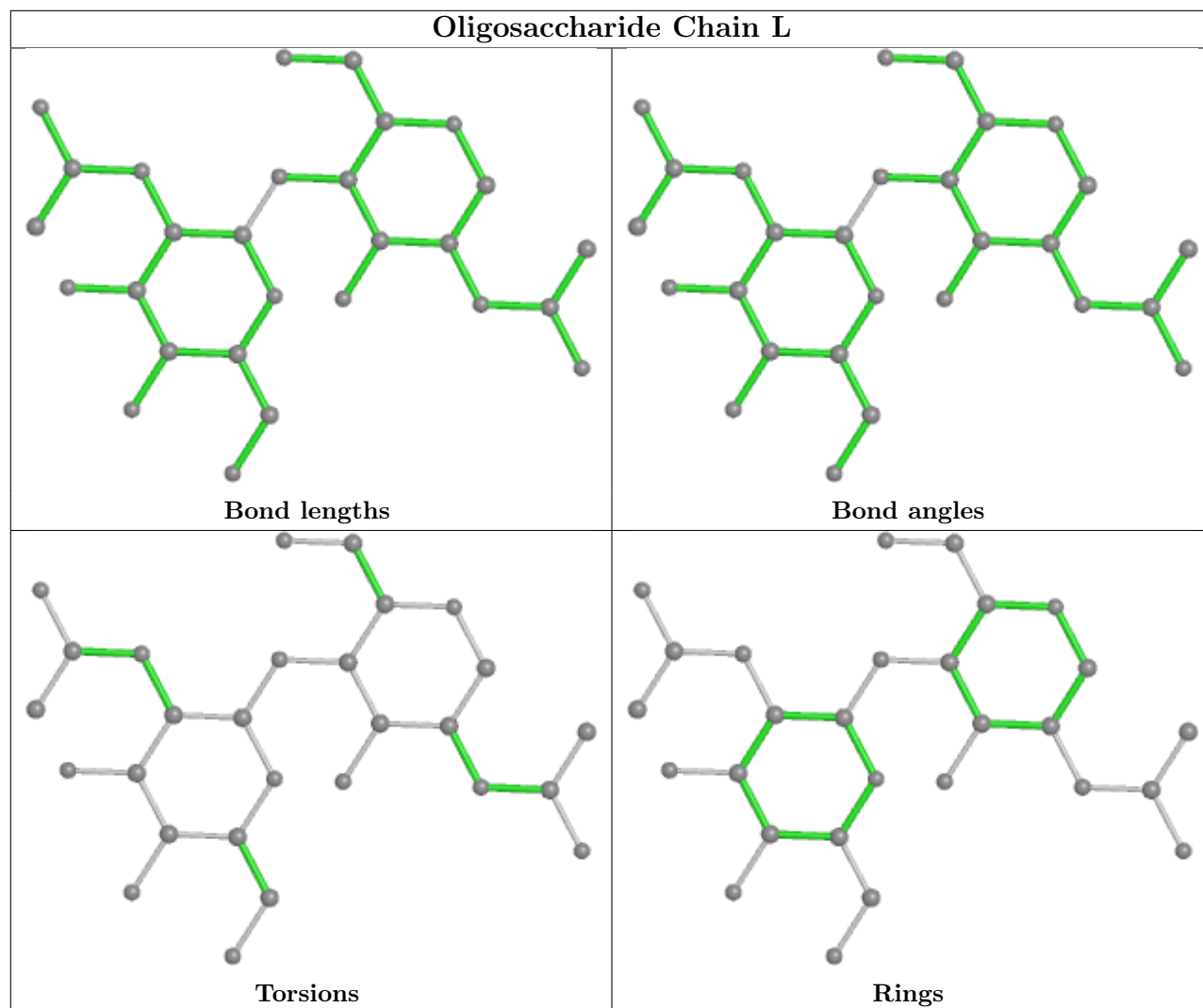


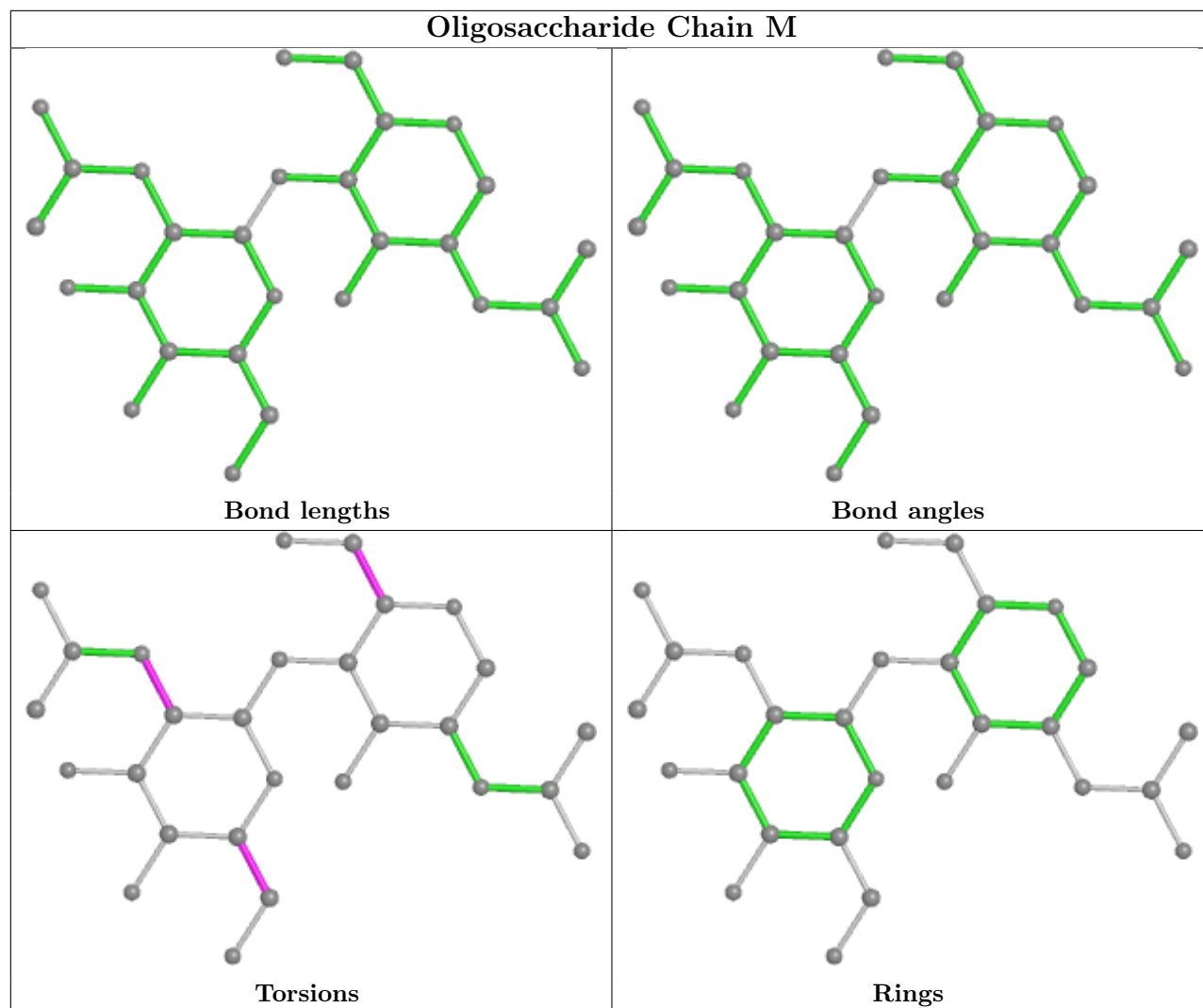


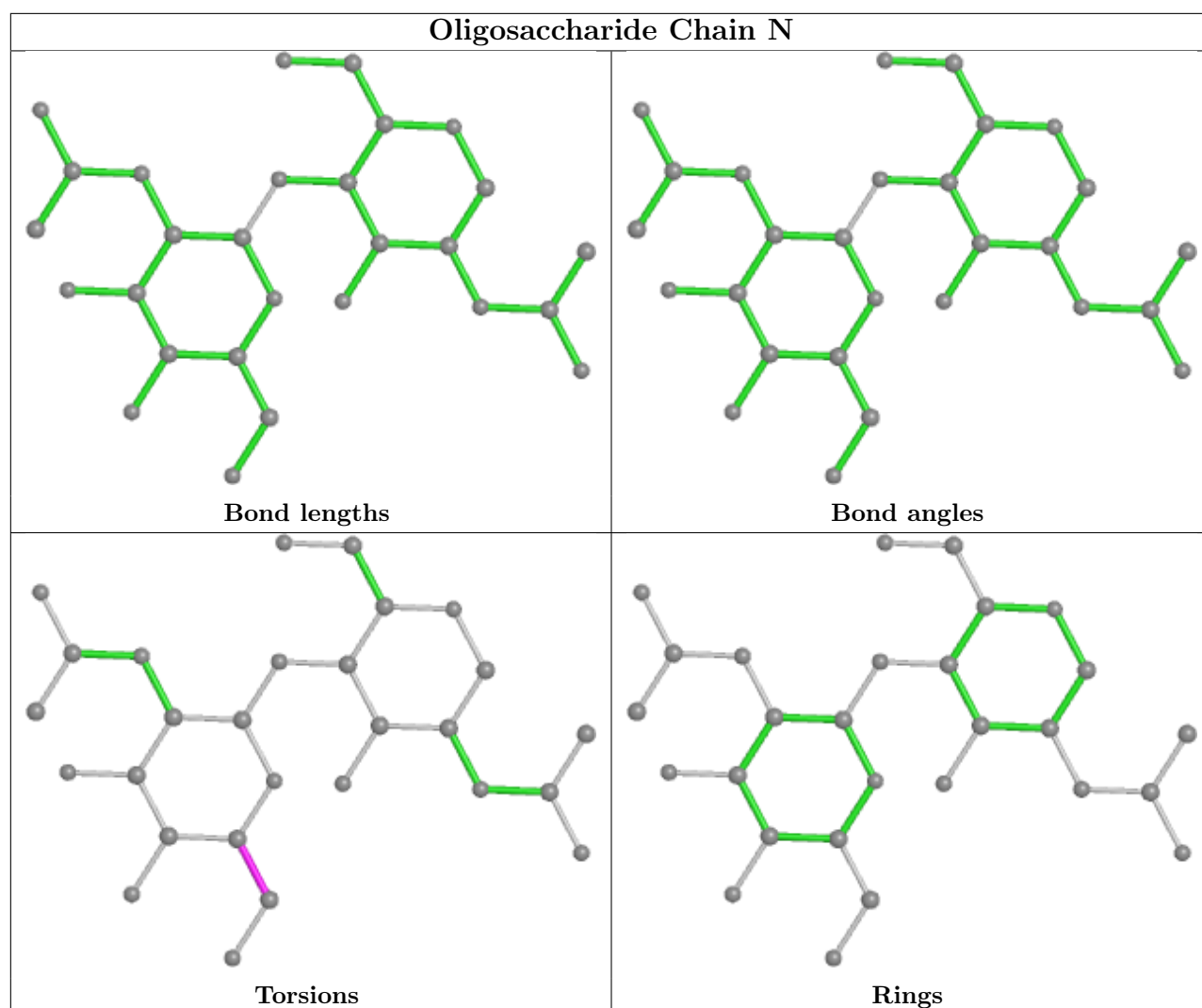


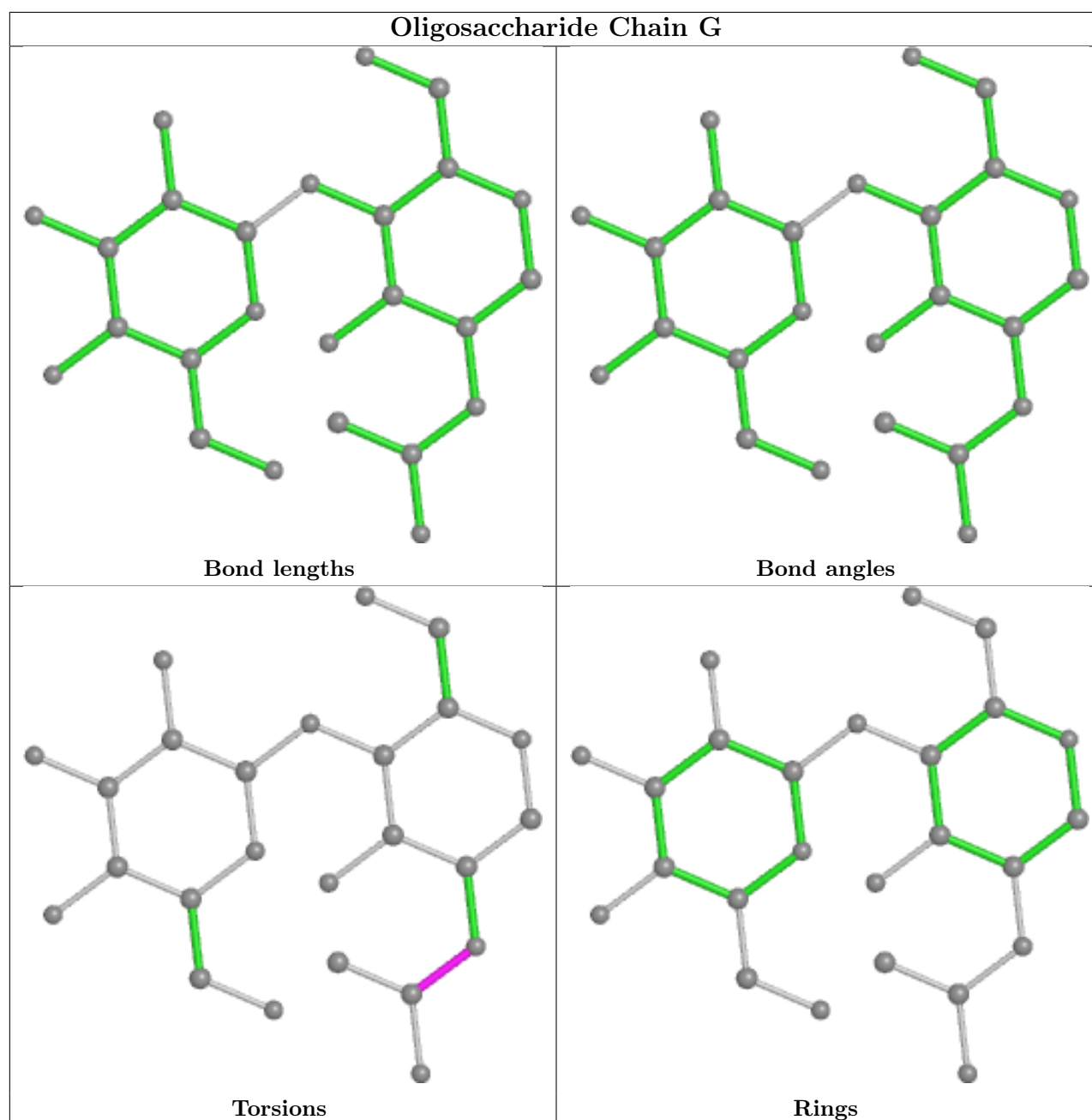












## 5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 for Mogul analysis.

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	501	1	14,14,15	0.20	0	17,19,21	0.41	0
5	NAG	B	1001	2	14,14,15	0.22	0	17,19,21	0.41	0
5	NAG	B	1002	2	14,14,15	0.20	0	17,19,21	0.42	0
5	NAG	D	1002	2	14,14,15	0.27	0	17,19,21	0.54	0
5	NAG	B	1003	2	14,14,15	0.22	0	17,19,21	0.43	0
5	NAG	C	501	1	14,14,15	0.19	0	17,19,21	0.40	0
5	NAG	D	1001	2	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
5	NAG	A	501	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1001	2	-	2/6/23/26	0/1/1/1
5	NAG	B	1002	2	-	3/6/23/26	0/1/1/1
5	NAG	D	1002	2	-	2/6/23/26	0/1/1/1
5	NAG	B	1003	2	-	2/6/23/26	0/1/1/1
5	NAG	C	501	1	-	0/6/23/26	0/1/1/1
5	NAG	D	1001	2	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	1001	NAG	C4-C5-C6-O6
5	D	1001	NAG	O5-C5-C6-O6
5	B	1001	NAG	C4-C5-C6-O6
5	D	1002	NAG	C4-C5-C6-O6
5	A	501	NAG	C8-C7-N2-C2
5	A	501	NAG	O7-C7-N2-C2
5	B	1002	NAG	C8-C7-N2-C2
5	B	1002	NAG	O7-C7-N2-C2
5	D	1001	NAG	C8-C7-N2-C2
5	D	1001	NAG	O7-C7-N2-C2
5	B	1001	NAG	O5-C5-C6-O6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
5	D	1002	NAG	O5-C5-C6-O6
5	B	1003	NAG	C4-C5-C6-O6
5	B	1003	NAG	O5-C5-C6-O6
5	B	1002	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	B	1002	NAG	1	0

## 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.