



Full wwPDB EM Validation Report ⓘ

Mar 26, 2026 – 08:10 PM UTC

PDB ID : 7MTE / pdb_00007mte
EMDB ID : EMD-23984
Title : Structure of SARS-CoV-2 S2P spike at pH 7.4 refolded by low-pH treatment
Authors : Tsybovsky, Y.; Olia, A.S.; Kwong, P.D.
Deposited on : 2021-05-13
Resolution : 3.20 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

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 : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
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

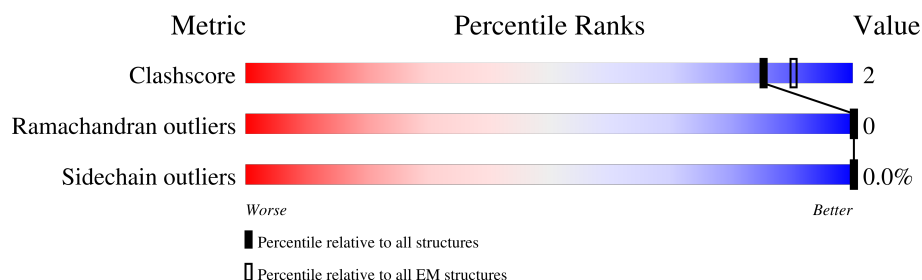
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 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 ≥ 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	1281	66% 30%
1	B	1281	58% 5% 37%
1	C	1281	64% 32%
2	D	2	100%
2	E	2	100%
2	F	2	50% 50%
2	G	2	100%
2	H	2	100%
2	I	2	50% 50%

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Mol	Chain	Length	Quality of chain
2	J	2	 100%
2	K	2	 50%50%
2	L	2	 100%
2	M	2	 100%
2	N	2	 100%
2	O	2	 50%50%
2	P	2	 50%50%
2	Q	2	 100%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 20612 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 glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	895	Total	C	N	O	S	0	0
			7002	4485	1159	1328	30		
1	B	802	Total	C	N	O	S	0	0
			6232	3987	1030	1190	25		
1	C	871	Total	C	N	O	S	0	0
			6790	4350	1122	1287	31		

There are 267 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	expression tag	UNP P0DTC2
A	-17	GLY	-	expression tag	UNP P0DTC2
A	-16	ILE	-	expression tag	UNP P0DTC2
A	-15	LEU	-	expression tag	UNP P0DTC2
A	-14	PRO	-	expression tag	UNP P0DTC2
A	-13	SER	-	expression tag	UNP P0DTC2
A	-12	PRO	-	expression tag	UNP P0DTC2
A	-11	GLY	-	expression tag	UNP P0DTC2
A	-10	MET	-	expression tag	UNP P0DTC2
A	-9	PRO	-	expression tag	UNP P0DTC2
A	-8	ALA	-	expression tag	UNP P0DTC2
A	-7	LEU	-	expression tag	UNP P0DTC2
A	-6	LEU	-	expression tag	UNP P0DTC2
A	-5	SER	-	expression tag	UNP P0DTC2
A	-4	LEU	-	expression tag	UNP P0DTC2
A	-3	VAL	-	expression tag	UNP P0DTC2
A	-2	SER	-	expression tag	UNP P0DTC2
A	-1	LEU	-	expression tag	UNP P0DTC2
A	0	LEU	-	expression tag	UNP P0DTC2
A	1	SER	-	expression tag	UNP P0DTC2
A	2	VAL	-	expression tag	UNP P0DTC2
A	3	LEU	-	expression tag	UNP P0DTC2
A	4	LEU	-	expression tag	UNP P0DTC2
A	5	MET	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	6	GLY	-	expression tag	UNP P0DTC2
A	7	CYS	-	expression tag	UNP P0DTC2
A	8	VAL	-	expression tag	UNP P0DTC2
A	9	ALA	-	expression tag	UNP P0DTC2
A	10	GLU	-	expression tag	UNP P0DTC2
A	11	THR	-	expression tag	UNP P0DTC2
A	12	GLY	-	expression tag	UNP P0DTC2
A	13	THR	-	expression tag	UNP P0DTC2
A	682	SER	ARG	conflict	UNP P0DTC2
A	683	GLY	ARG	conflict	UNP P0DTC2
A	685	GLY	ARG	conflict	UNP P0DTC2
A	829	ILE	ALA	conflict	UNP P0DTC2
A	986	PRO	LYS	conflict	UNP P0DTC2
A	987	PRO	VAL	conflict	UNP P0DTC2
A	1212	GLY	-	expression tag	UNP P0DTC2
A	1213	SER	-	expression tag	UNP P0DTC2
A	1214	GLY	-	expression tag	UNP P0DTC2
A	1215	ARG	-	expression tag	UNP P0DTC2
A	1216	GLU	-	expression tag	UNP P0DTC2
A	1217	ASN	-	expression tag	UNP P0DTC2
A	1218	LEU	-	expression tag	UNP P0DTC2
A	1219	TYR	-	expression tag	UNP P0DTC2
A	1220	PHE	-	expression tag	UNP P0DTC2
A	1221	GLN	-	expression tag	UNP P0DTC2
A	1222	GLY	-	expression tag	UNP P0DTC2
A	1223	GLY	-	expression tag	UNP P0DTC2
A	1224	GLY	-	expression tag	UNP P0DTC2
A	1225	GLY	-	expression tag	UNP P0DTC2
A	1226	SER	-	expression tag	UNP P0DTC2
A	1227	GLY	-	expression tag	UNP P0DTC2
A	1228	TYR	-	expression tag	UNP P0DTC2
A	1229	ILE	-	expression tag	UNP P0DTC2
A	1230	PRO	-	expression tag	UNP P0DTC2
A	1231	GLU	-	expression tag	UNP P0DTC2
A	1232	ALA	-	expression tag	UNP P0DTC2
A	1233	PRO	-	expression tag	UNP P0DTC2
A	1234	ARG	-	expression tag	UNP P0DTC2
A	1235	ASP	-	expression tag	UNP P0DTC2
A	1236	GLY	-	expression tag	UNP P0DTC2
A	1237	GLN	-	expression tag	UNP P0DTC2
A	1238	ALA	-	expression tag	UNP P0DTC2
A	1239	TYR	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1240	VAL	-	expression tag	UNP P0DTC2
A	1241	ARG	-	expression tag	UNP P0DTC2
A	1242	LYS	-	expression tag	UNP P0DTC2
A	1243	ASP	-	expression tag	UNP P0DTC2
A	1244	GLY	-	expression tag	UNP P0DTC2
A	1245	GLU	-	expression tag	UNP P0DTC2
A	1246	TRP	-	expression tag	UNP P0DTC2
A	1247	VAL	-	expression tag	UNP P0DTC2
A	1248	LEU	-	expression tag	UNP P0DTC2
A	1249	LEU	-	expression tag	UNP P0DTC2
A	1250	SER	-	expression tag	UNP P0DTC2
A	1251	THR	-	expression tag	UNP P0DTC2
A	1252	PHE	-	expression tag	UNP P0DTC2
A	1253	LEU	-	expression tag	UNP P0DTC2
A	1254	GLY	-	expression tag	UNP P0DTC2
A	1255	HIS	-	expression tag	UNP P0DTC2
A	1256	HIS	-	expression tag	UNP P0DTC2
A	1257	HIS	-	expression tag	UNP P0DTC2
A	1258	HIS	-	expression tag	UNP P0DTC2
A	1259	HIS	-	expression tag	UNP P0DTC2
A	1260	HIS	-	expression tag	UNP P0DTC2
A	1261	HIS	-	expression tag	UNP P0DTC2
A	1262	HIS	-	expression tag	UNP P0DTC2
B	-18	MET	-	expression tag	UNP P0DTC2
B	-17	GLY	-	expression tag	UNP P0DTC2
B	-16	ILE	-	expression tag	UNP P0DTC2
B	-15	LEU	-	expression tag	UNP P0DTC2
B	-14	PRO	-	expression tag	UNP P0DTC2
B	-13	SER	-	expression tag	UNP P0DTC2
B	-12	PRO	-	expression tag	UNP P0DTC2
B	-11	GLY	-	expression tag	UNP P0DTC2
B	-10	MET	-	expression tag	UNP P0DTC2
B	-9	PRO	-	expression tag	UNP P0DTC2
B	-8	ALA	-	expression tag	UNP P0DTC2
B	-7	LEU	-	expression tag	UNP P0DTC2
B	-6	LEU	-	expression tag	UNP P0DTC2
B	-5	SER	-	expression tag	UNP P0DTC2
B	-4	LEU	-	expression tag	UNP P0DTC2
B	-3	VAL	-	expression tag	UNP P0DTC2
B	-2	SER	-	expression tag	UNP P0DTC2
B	-1	LEU	-	expression tag	UNP P0DTC2
B	0	LEU	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1	SER	-	expression tag	UNP P0DTC2
B	2	VAL	-	expression tag	UNP P0DTC2
B	3	LEU	-	expression tag	UNP P0DTC2
B	4	LEU	-	expression tag	UNP P0DTC2
B	5	MET	-	expression tag	UNP P0DTC2
B	6	GLY	-	expression tag	UNP P0DTC2
B	7	CYS	-	expression tag	UNP P0DTC2
B	8	VAL	-	expression tag	UNP P0DTC2
B	9	ALA	-	expression tag	UNP P0DTC2
B	10	GLU	-	expression tag	UNP P0DTC2
B	11	THR	-	expression tag	UNP P0DTC2
B	12	GLY	-	expression tag	UNP P0DTC2
B	13	THR	-	expression tag	UNP P0DTC2
B	682	SER	ARG	conflict	UNP P0DTC2
B	683	GLY	ARG	conflict	UNP P0DTC2
B	685	GLY	ARG	conflict	UNP P0DTC2
B	829	ILE	ALA	conflict	UNP P0DTC2
B	986	PRO	LYS	conflict	UNP P0DTC2
B	987	PRO	VAL	conflict	UNP P0DTC2
B	1212	GLY	-	expression tag	UNP P0DTC2
B	1213	SER	-	expression tag	UNP P0DTC2
B	1214	GLY	-	expression tag	UNP P0DTC2
B	1215	ARG	-	expression tag	UNP P0DTC2
B	1216	GLU	-	expression tag	UNP P0DTC2
B	1217	ASN	-	expression tag	UNP P0DTC2
B	1218	LEU	-	expression tag	UNP P0DTC2
B	1219	TYR	-	expression tag	UNP P0DTC2
B	1220	PHE	-	expression tag	UNP P0DTC2
B	1221	GLN	-	expression tag	UNP P0DTC2
B	1222	GLY	-	expression tag	UNP P0DTC2
B	1223	GLY	-	expression tag	UNP P0DTC2
B	1224	GLY	-	expression tag	UNP P0DTC2
B	1225	GLY	-	expression tag	UNP P0DTC2
B	1226	SER	-	expression tag	UNP P0DTC2
B	1227	GLY	-	expression tag	UNP P0DTC2
B	1228	TYR	-	expression tag	UNP P0DTC2
B	1229	ILE	-	expression tag	UNP P0DTC2
B	1230	PRO	-	expression tag	UNP P0DTC2
B	1231	GLU	-	expression tag	UNP P0DTC2
B	1232	ALA	-	expression tag	UNP P0DTC2
B	1233	PRO	-	expression tag	UNP P0DTC2
B	1234	ARG	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1235	ASP	-	expression tag	UNP P0DTC2
B	1236	GLY	-	expression tag	UNP P0DTC2
B	1237	GLN	-	expression tag	UNP P0DTC2
B	1238	ALA	-	expression tag	UNP P0DTC2
B	1239	TYR	-	expression tag	UNP P0DTC2
B	1240	VAL	-	expression tag	UNP P0DTC2
B	1241	ARG	-	expression tag	UNP P0DTC2
B	1242	LYS	-	expression tag	UNP P0DTC2
B	1243	ASP	-	expression tag	UNP P0DTC2
B	1244	GLY	-	expression tag	UNP P0DTC2
B	1245	GLU	-	expression tag	UNP P0DTC2
B	1246	TRP	-	expression tag	UNP P0DTC2
B	1247	VAL	-	expression tag	UNP P0DTC2
B	1248	LEU	-	expression tag	UNP P0DTC2
B	1249	LEU	-	expression tag	UNP P0DTC2
B	1250	SER	-	expression tag	UNP P0DTC2
B	1251	THR	-	expression tag	UNP P0DTC2
B	1252	PHE	-	expression tag	UNP P0DTC2
B	1253	LEU	-	expression tag	UNP P0DTC2
B	1254	GLY	-	expression tag	UNP P0DTC2
B	1255	HIS	-	expression tag	UNP P0DTC2
B	1256	HIS	-	expression tag	UNP P0DTC2
B	1257	HIS	-	expression tag	UNP P0DTC2
B	1258	HIS	-	expression tag	UNP P0DTC2
B	1259	HIS	-	expression tag	UNP P0DTC2
B	1260	HIS	-	expression tag	UNP P0DTC2
B	1261	HIS	-	expression tag	UNP P0DTC2
B	1262	HIS	-	expression tag	UNP P0DTC2
C	-18	MET	-	expression tag	UNP P0DTC2
C	-17	GLY	-	expression tag	UNP P0DTC2
C	-16	ILE	-	expression tag	UNP P0DTC2
C	-15	LEU	-	expression tag	UNP P0DTC2
C	-14	PRO	-	expression tag	UNP P0DTC2
C	-13	SER	-	expression tag	UNP P0DTC2
C	-12	PRO	-	expression tag	UNP P0DTC2
C	-11	GLY	-	expression tag	UNP P0DTC2
C	-10	MET	-	expression tag	UNP P0DTC2
C	-9	PRO	-	expression tag	UNP P0DTC2
C	-8	ALA	-	expression tag	UNP P0DTC2
C	-7	LEU	-	expression tag	UNP P0DTC2
C	-6	LEU	-	expression tag	UNP P0DTC2
C	-5	SER	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	LEU	-	expression tag	UNP P0DTC2
C	-3	VAL	-	expression tag	UNP P0DTC2
C	-2	SER	-	expression tag	UNP P0DTC2
C	-1	LEU	-	expression tag	UNP P0DTC2
C	0	LEU	-	expression tag	UNP P0DTC2
C	1	SER	-	expression tag	UNP P0DTC2
C	2	VAL	-	expression tag	UNP P0DTC2
C	3	LEU	-	expression tag	UNP P0DTC2
C	4	LEU	-	expression tag	UNP P0DTC2
C	5	MET	-	expression tag	UNP P0DTC2
C	6	GLY	-	expression tag	UNP P0DTC2
C	7	CYS	-	expression tag	UNP P0DTC2
C	8	VAL	-	expression tag	UNP P0DTC2
C	9	ALA	-	expression tag	UNP P0DTC2
C	10	GLU	-	expression tag	UNP P0DTC2
C	11	THR	-	expression tag	UNP P0DTC2
C	12	GLY	-	expression tag	UNP P0DTC2
C	13	THR	-	expression tag	UNP P0DTC2
C	682	SER	ARG	conflict	UNP P0DTC2
C	683	GLY	ARG	conflict	UNP P0DTC2
C	685	GLY	ARG	conflict	UNP P0DTC2
C	829	ILE	ALA	conflict	UNP P0DTC2
C	986	PRO	LYS	conflict	UNP P0DTC2
C	987	PRO	VAL	conflict	UNP P0DTC2
C	1212	GLY	-	expression tag	UNP P0DTC2
C	1213	SER	-	expression tag	UNP P0DTC2
C	1214	GLY	-	expression tag	UNP P0DTC2
C	1215	ARG	-	expression tag	UNP P0DTC2
C	1216	GLU	-	expression tag	UNP P0DTC2
C	1217	ASN	-	expression tag	UNP P0DTC2
C	1218	LEU	-	expression tag	UNP P0DTC2
C	1219	TYR	-	expression tag	UNP P0DTC2
C	1220	PHE	-	expression tag	UNP P0DTC2
C	1221	GLN	-	expression tag	UNP P0DTC2
C	1222	GLY	-	expression tag	UNP P0DTC2
C	1223	GLY	-	expression tag	UNP P0DTC2
C	1224	GLY	-	expression tag	UNP P0DTC2
C	1225	GLY	-	expression tag	UNP P0DTC2
C	1226	SER	-	expression tag	UNP P0DTC2
C	1227	GLY	-	expression tag	UNP P0DTC2
C	1228	TYR	-	expression tag	UNP P0DTC2
C	1229	ILE	-	expression tag	UNP P0DTC2

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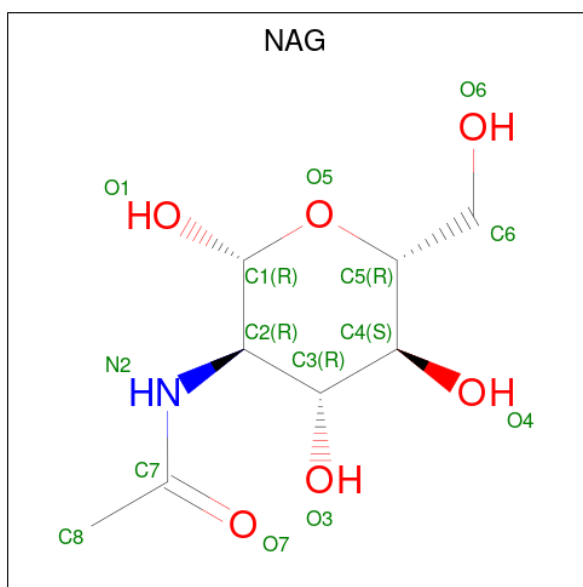
Chain	Residue	Modelled	Actual	Comment	Reference
C	1230	PRO	-	expression tag	UNP P0DTC2
C	1231	GLU	-	expression tag	UNP P0DTC2
C	1232	ALA	-	expression tag	UNP P0DTC2
C	1233	PRO	-	expression tag	UNP P0DTC2
C	1234	ARG	-	expression tag	UNP P0DTC2
C	1235	ASP	-	expression tag	UNP P0DTC2
C	1236	GLY	-	expression tag	UNP P0DTC2
C	1237	GLN	-	expression tag	UNP P0DTC2
C	1238	ALA	-	expression tag	UNP P0DTC2
C	1239	TYR	-	expression tag	UNP P0DTC2
C	1240	VAL	-	expression tag	UNP P0DTC2
C	1241	ARG	-	expression tag	UNP P0DTC2
C	1242	LYS	-	expression tag	UNP P0DTC2
C	1243	ASP	-	expression tag	UNP P0DTC2
C	1244	GLY	-	expression tag	UNP P0DTC2
C	1245	GLU	-	expression tag	UNP P0DTC2
C	1246	TRP	-	expression tag	UNP P0DTC2
C	1247	VAL	-	expression tag	UNP P0DTC2
C	1248	LEU	-	expression tag	UNP P0DTC2
C	1249	LEU	-	expression tag	UNP P0DTC2
C	1250	SER	-	expression tag	UNP P0DTC2
C	1251	THR	-	expression tag	UNP P0DTC2
C	1252	PHE	-	expression tag	UNP P0DTC2
C	1253	LEU	-	expression tag	UNP P0DTC2
C	1254	GLY	-	expression tag	UNP P0DTC2
C	1255	HIS	-	expression tag	UNP P0DTC2
C	1256	HIS	-	expression tag	UNP P0DTC2
C	1257	HIS	-	expression tag	UNP P0DTC2
C	1258	HIS	-	expression tag	UNP P0DTC2
C	1259	HIS	-	expression tag	UNP P0DTC2
C	1260	HIS	-	expression tag	UNP P0DTC2
C	1261	HIS	-	expression tag	UNP P0DTC2
C	1262	HIS	-	expression tag	UNP P0DTC2

- Molecule 2 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
2	D	2	Total	C	N	O	0	0
			28	16	2	10		
2	E	2	Total	C	N	O	0	0
			28	16	2	10		
2	F	2	Total	C	N	O	0	0
			28	16	2	10		
2	G	2	Total	C	N	O	0	0
			28	16	2	10		
2	H	2	Total	C	N	O	0	0
			28	16	2	10		
2	I	2	Total	C	N	O	0	0
			28	16	2	10		
2	J	2	Total	C	N	O	0	0
			28	16	2	10		
2	K	2	Total	C	N	O	0	0
			28	16	2	10		
2	L	2	Total	C	N	O	0	0
			28	16	2	10		
2	M	2	Total	C	N	O	0	0
			28	16	2	10		
2	N	2	Total	C	N	O	0	0
			28	16	2	10		
2	O	2	Total	C	N	O	0	0
			28	16	2	10		
2	P	2	Total	C	N	O	0	0
			28	16	2	10		
2	Q	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

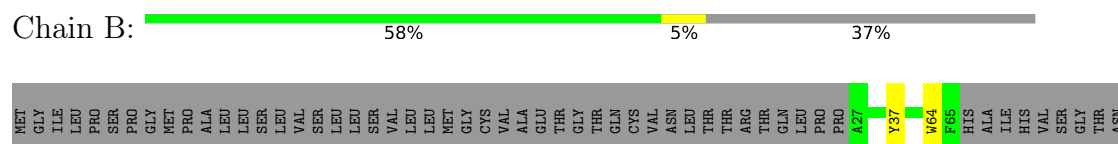
3 Residue-property plots

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.

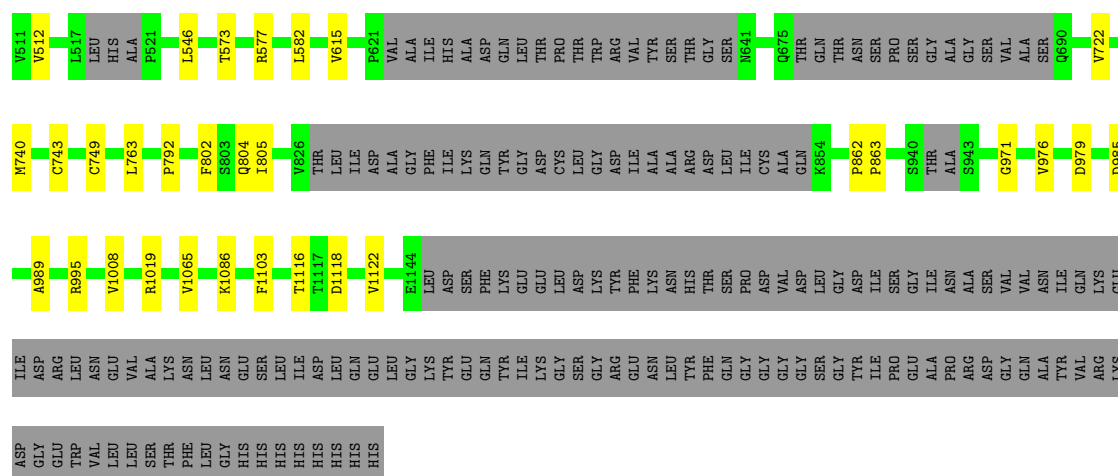
• Molecule 1: Spike glycoprotein



• Molecule 1: Spike glycoprotein







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

Chain D:  100%



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

Chain E:  100%



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

Chain F:  50% 50%



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

Chain G:  100%



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

Chain H:  100%



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

Chain I:  50% 50%



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

Chain J:  100%



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

Chain K:  50% 50%



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

Chain L:  100%



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

Chain M:  100%



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

Chain N:  100%



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

Chain O:  50% 50%

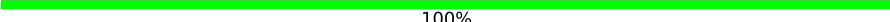
MAG1
MAG2

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

Chain P:  50% 50%

MAG1
MAG2

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

Chain Q:  100%

MAG1
MAG2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	252067	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (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: 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	0.19	0/7149	0.47	2/9710 (0.0%)
1	B	0.20	0/6360	0.46	0/8653
1	C	0.19	0/6934	0.47	2/9424 (0.0%)
All	All	0.19	0/20443	0.47	4/27787 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	31	SER	CA-C-N	5.70	132.43	121.54
1	C	31	SER	C-N-CA	5.70	132.43	121.54
1	A	744	GLY	CA-C-N	5.06	131.21	121.54
1	A	744	GLY	C-N-CA	5.06	131.21	121.54

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	361	CYS	Peptide

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Mol	Chain	Res	Type	Group
1	B	904	TYR	Peptide

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	7002	0	6864	27	0
1	B	6232	0	6137	36	0
1	C	6790	0	6657	31	0
2	D	28	0	25	0	0
2	E	28	0	25	0	0
2	F	28	0	25	0	0
2	G	28	0	25	0	0
2	H	28	0	25	0	0
2	I	28	0	25	0	0
2	J	28	0	25	0	0
2	K	28	0	25	0	0
2	L	28	0	25	0	0
2	M	28	0	25	0	0
2	N	28	0	25	0	0
2	O	28	0	25	1	0
2	P	28	0	25	1	0
2	Q	28	0	25	0	0
3	A	56	0	52	0	0
3	B	84	0	78	0	0
3	C	56	0	52	0	0
All	All	20612	0	20190	91	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 2.

All (91) 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:C:336:CYS:H	1:C:363:ALA:HB2	1.60	0.66
1:A:403:ARG:HG3	1:A:405:ASP:H	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:546:LEU:HD11	1:C:573:THR:HG21	1.85	0.59
1:A:106:PHE:HB2	1:A:117:LEU:HB3	1.86	0.57
1:C:65:PHE:O	1:C:264:ALA:N	2.38	0.57
1:B:814:LYS:HE3	1:B:872:GLN:HG2	1.88	0.55
1:A:329:PHE:O	1:A:580:GLN:NE2	2.38	0.54
1:A:722:VAL:HG22	1:A:1065:VAL:HG22	1.90	0.54
1:A:525:CYS:SG	1:A:526:GLY:N	2.80	0.54
1:B:624:ILE:HD11	1:B:637:SER:HB3	1.90	0.53
1:C:971:GLY:HA3	1:C:995:ARG:HH21	1.73	0.53
1:A:57:PRO:HG3	1:A:273:ARG:HE	1.73	0.53
1:C:398:ASP:HB2	1:C:512:VAL:HB	1.90	0.53
1:B:319:ARG:HE	1:C:740:MET:HE2	1.75	0.52
1:B:106:PHE:HB2	1:B:117:LEU:HB3	1.91	0.52
1:B:971:GLY:O	1:B:995:ARG:NH1	2.43	0.52
1:A:1047:TYR:HB2	1:A:1067:TYR:HB3	1.93	0.51
1:B:707:TYR:HB3	1:C:792:PRO:HG2	1.93	0.51
1:B:37:TYR:OH	1:B:195:LYS:NZ	2.38	0.51
1:B:1017:GLU:OE1	1:C:1019:ARG:NH1	2.41	0.50
1:C:1103:PHE:HZ	2:P:1:NAG:H62	1.76	0.50
1:C:318:PHE:HZ	1:C:615:VAL:HG21	1.75	0.50
1:C:577:ARG:HD3	1:C:582:LEU:HD22	1.93	0.49
1:A:193:VAL:HB	1:A:204:TYR:HB2	1.93	0.49
1:A:318:PHE:HZ	1:A:615:VAL:HG11	1.77	0.49
1:B:722:VAL:HG22	1:B:1065:VAL:HG22	1.95	0.49
1:B:106:PHE:HD2	1:B:117:LEU:HD23	1.78	0.49
1:B:717:ASN:HB3	1:B:1070:ALA:HB3	1.94	0.48
1:A:715:PRO:HA	1:A:1072:GLU:HA	1.95	0.48
1:B:64:TRP:HD1	1:B:266:TYR:HE1	1.59	0.48
1:C:976:VAL:HG12	1:C:979:ASP:H	1.79	0.47
1:B:811:LYS:NZ	1:B:820:ASP:OD2	2.34	0.46
1:A:802:PHE:HD1	1:A:805:ILE:HD11	1.80	0.46
1:B:91:TYR:OH	1:B:191:GLU:OE1	2.30	0.46
1:B:828:LEU:HB2	1:B:949:GLN:HE22	1.80	0.46
1:C:985:ASP:O	1:C:989:ALA:HB2	2.17	0.45
1:B:624:ILE:HD12	1:B:633:TRP:HE1	1.83	0.44
1:B:1030:SER:HA	1:B:1034:LEU:HD12	1.99	0.44
1:C:64:TRP:HE1	1:C:66:HIS:CE1	2.36	0.44
1:B:666:ILE:HD11	1:B:672:ALA:HB2	2.00	0.44
1:B:540:ASN:ND2	1:B:549:THR:OG1	2.50	0.44
1:A:522:ALA:HB1	1:A:525:CYS:HB2	2.00	0.44
1:B:659:SER:HB3	1:B:698:SER:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:722:VAL:HG22	1:C:1065:VAL:HG22	1.99	0.44
1:B:385:THR:HG23	1:B:386:LYS:HG3	1.99	0.44
1:B:880:GLY:O	1:B:884:SER:OG	2.33	0.44
1:B:108:THR:HG22	1:B:109:THR:HG23	2.00	0.43
1:C:54:LEU:HD12	1:C:195:LYS:HD2	2.00	0.43
1:C:804:GLN:NE2	2:O:1:NAG:O6	2.51	0.43
1:A:402:ILE:HG23	1:A:404:GLY:H	1.83	0.43
1:B:198:ASP:OD1	1:B:198:ASP:N	2.51	0.43
1:C:44:ARG:HB2	1:C:279:TYR:CD2	2.54	0.43
1:C:763:LEU:HD22	1:C:1008:VAL:HG21	2.01	0.43
1:C:106:PHE:HB2	1:C:117:LEU:HB3	2.00	0.43
1:C:353:TRP:H	1:C:466:ARG:HH22	1.65	0.43
1:B:763:LEU:HD22	1:B:1008:VAL:HG21	2.00	0.43
1:C:462:LYS:HB2	1:C:465:GLU:HB2	2.01	0.42
1:A:743:CYS:HB3	1:A:749:CYS:HB3	1.84	0.42
1:A:565:PHE:HA	1:A:576:VAL:HA	2.01	0.42
1:A:280:ASN:OD1	1:A:284:THR:N	2.47	0.42
1:A:461:LEU:HD23	1:A:465:GLU:HB3	2.01	0.42
1:B:314:GLN:NE2	1:B:316:SER:O	2.53	0.42
1:A:945:LEU:HD23	1:A:948:LEU:HD12	2.01	0.42
1:A:402:ILE:HG22	1:A:510:VAL:HG21	2.01	0.42
1:A:376:THR:HB	1:A:435:ALA:HB3	2.01	0.41
1:B:615:VAL:HG12	1:B:617:CYS:H	1.85	0.41
1:C:802:PHE:HD1	1:C:805:ILE:HD11	1.85	0.41
1:A:594:GLY:H	1:A:613:GLN:HB2	1.84	0.41
1:C:1086:LYS:HD3	1:C:1122:VAL:HG11	2.02	0.41
1:C:862:PRO:HA	1:C:863:PRO:HD3	1.96	0.41
1:C:89:GLY:HA3	1:C:270:LEU:HD12	2.02	0.41
1:B:1116:THR:HG22	1:B:1138:TYR:HB3	2.03	0.41
1:C:985:ASP:O	1:C:989:ALA:CB	2.69	0.41
1:A:206:LYS:HB3	1:A:223:LEU:HG	2.01	0.41
1:A:763:LEU:HD22	1:A:1008:VAL:HG21	2.03	0.41
1:C:1116:THR:OG1	1:C:1118:ASP:OD1	2.31	0.41
1:B:83:VAL:HG11	1:B:237:ARG:HH11	1.86	0.41
1:B:725:GLU:OE1	1:B:1064:HIS:NE2	2.50	0.41
1:B:383:SER:HA	1:B:384:PRO:HD3	1.94	0.41
1:C:84:LEU:HD22	1:C:267:VAL:HG21	2.03	0.41
1:C:743:CYS:HB3	1:C:749:CYS:HB3	1.84	0.41
1:A:326:ILE:HD12	1:A:326:ILE:HA	1.96	0.41
1:B:197:ILE:HD11	1:B:200:TYR:HB2	2.02	0.41
1:B:316:SER:OG	1:B:317:ASN:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:LYS:H	1:A:41:LYS:HD2	1.85	0.40
1:A:120:VAL:HG12	1:A:241:LEU:HD11	2.03	0.40
1:A:280:ASN:ND2	1:A:284:THR:OG1	2.51	0.40
1:B:605:SER:OG	1:B:606:ASN:N	2.53	0.40
1:B:742:ILE:O	1:B:1000:ARG:NH1	2.46	0.40
1:C:193:VAL:HG23	1:C:223:LEU:HD22	2.03	0.40
1:B:825:LYS:NZ	1:B:942:ALA:O	2.41	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	859/1281 (67%)	817 (95%)	42 (5%)	0	100	100
1	B	774/1281 (60%)	747 (96%)	27 (4%)	0	100	100
1	C	837/1281 (65%)	795 (95%)	42 (5%)	0	100	100
All	All	2470/3843 (64%)	2359 (96%)	111 (4%)	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	785/1108 (71%)	784 (100%)	1 (0%)	88	91
1	B	704/1108 (64%)	704 (100%)	0	100	100
1	C	762/1108 (69%)	762 (100%)	0	100	100
All	All	2251/3324 (68%)	2250 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	524	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	HIS
1	A	354	ASN
1	A	493	GLN
1	A	564	GLN
1	A	764	ASN
1	A	901	GLN
1	A	992	GLN
1	A	1011	GLN
1	B	540	ASN
1	B	779	GLN
1	B	901	GLN
1	B	949	GLN
1	B	992	GLN
1	B	1002	GLN
1	B	1135	ASN
1	C	234	ASN
1	C	354	ASN
1	C	370	ASN
1	C	644	GLN
1	C	804	GLN
1	C	901	GLN
1	C	926	GLN
1	C	935	GLN
1	C	953	ASN
1	C	992	GLN
1	C	1005	GLN
1	C	1071	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 ⓘ

28 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	$\# Z > 2$
2	NAG	D	1	1,2	14,14,15	0.22	0	17,19,21	0.56	0
2	NAG	D	2	2	14,14,15	0.39	0	17,19,21	0.45	0
2	NAG	E	1	1,2	14,14,15	0.30	0	17,19,21	0.56	0
2	NAG	E	2	2	14,14,15	0.31	0	17,19,21	0.49	0
2	NAG	F	1	1,2	14,14,15	0.47	0	17,19,21	0.76	1 (5%)
2	NAG	F	2	2	14,14,15	0.31	0	17,19,21	0.46	0
2	NAG	G	1	1,2	14,14,15	0.24	0	17,19,21	0.52	0
2	NAG	G	2	2	14,14,15	0.32	0	17,19,21	0.47	0
2	NAG	H	1	1,2	14,14,15	0.27	0	17,19,21	0.61	0
2	NAG	H	2	2	14,14,15	0.44	0	17,19,21	0.41	0
2	NAG	I	1	1,2	14,14,15	0.24	0	17,19,21	0.61	0
2	NAG	I	2	2	14,14,15	0.54	0	17,19,21	1.02	1 (5%)
2	NAG	J	1	1,2	14,14,15	0.31	0	17,19,21	0.53	0
2	NAG	J	2	2	14,14,15	0.34	0	17,19,21	0.47	0
2	NAG	K	1	1,2	14,14,15	0.28	0	17,19,21	0.52	0
2	NAG	K	2	2	14,14,15	0.41	0	17,19,21	0.66	1 (5%)
2	NAG	L	1	1,2	14,14,15	0.30	0	17,19,21	0.54	0
2	NAG	L	2	2	14,14,15	0.36	0	17,19,21	0.51	0
2	NAG	M	1	1,2	14,14,15	0.24	0	17,19,21	0.59	0
2	NAG	M	2	2	14,14,15	0.48	0	17,19,21	0.44	0
2	NAG	N	1	1,2	14,14,15	0.29	0	17,19,21	0.60	0
2	NAG	N	2	2	14,14,15	0.42	0	17,19,21	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	O	1	1,2	14,14,15	0.34	0	17,19,21	0.68	1 (5%)
2	NAG	O	2	2	14,14,15	0.41	0	17,19,21	0.44	0
2	NAG	P	1	1,2	14,14,15	0.25	0	17,19,21	0.56	0
2	NAG	P	2	2	14,14,15	0.37	0	17,19,21	0.49	0
2	NAG	Q	1	1,2	14,14,15	0.27	0	17,19,21	0.56	0
2	NAG	Q	2	2	14,14,15	0.32	0	17,19,21	0.52	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
2	NAG	D	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	NAG	E	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1
2	NAG	G	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	G	2	2	-	2/6/23/26	0/1/1/1
2	NAG	H	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	2/6/23/26	0/1/1/1
2	NAG	I	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	I	2	2	-	4/6/23/26	0/1/1/1
2	NAG	J	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	J	2	2	-	0/6/23/26	0/1/1/1
2	NAG	K	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	K	2	2	-	0/6/23/26	0/1/1/1
2	NAG	L	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	L	2	2	-	1/6/23/26	0/1/1/1
2	NAG	M	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	M	2	2	-	2/6/23/26	0/1/1/1
2	NAG	N	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	N	2	2	-	2/6/23/26	0/1/1/1
2	NAG	O	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	O	2	2	-	2/6/23/26	0/1/1/1
2	NAG	P	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	P	2	2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	Q	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	Q	2	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	2	NAG	C2-N2-C7	3.28	127.30	122.90
2	F	1	NAG	C1-O5-C5	2.48	115.52	112.19
2	K	2	NAG	C1-O5-C5	2.31	115.28	112.19
2	O	1	NAG	C1-O5-C5	2.12	115.03	112.19

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	M	2	NAG	O5-C5-C6-O6
2	F	2	NAG	O5-C5-C6-O6
2	Q	2	NAG	C4-C5-C6-O6
2	O	2	NAG	O5-C5-C6-O6
2	I	2	NAG	C4-C5-C6-O6
2	Q	2	NAG	O5-C5-C6-O6
2	O	2	NAG	C4-C5-C6-O6
2	G	2	NAG	O5-C5-C6-O6
2	F	2	NAG	C4-C5-C6-O6
2	M	2	NAG	C4-C5-C6-O6
2	G	2	NAG	C4-C5-C6-O6
2	Q	1	NAG	O5-C5-C6-O6
2	I	1	NAG	C8-C7-N2-C2
2	I	1	NAG	O7-C7-N2-C2
2	D	2	NAG	O5-C5-C6-O6
2	N	1	NAG	C4-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
2	N	2	NAG	C4-C5-C6-O6
2	I	2	NAG	O5-C5-C6-O6
2	H	2	NAG	O5-C5-C6-O6
2	H	2	NAG	C4-C5-C6-O6
2	N	1	NAG	O5-C5-C6-O6
2	N	2	NAG	O5-C5-C6-O6
2	G	1	NAG	O5-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6

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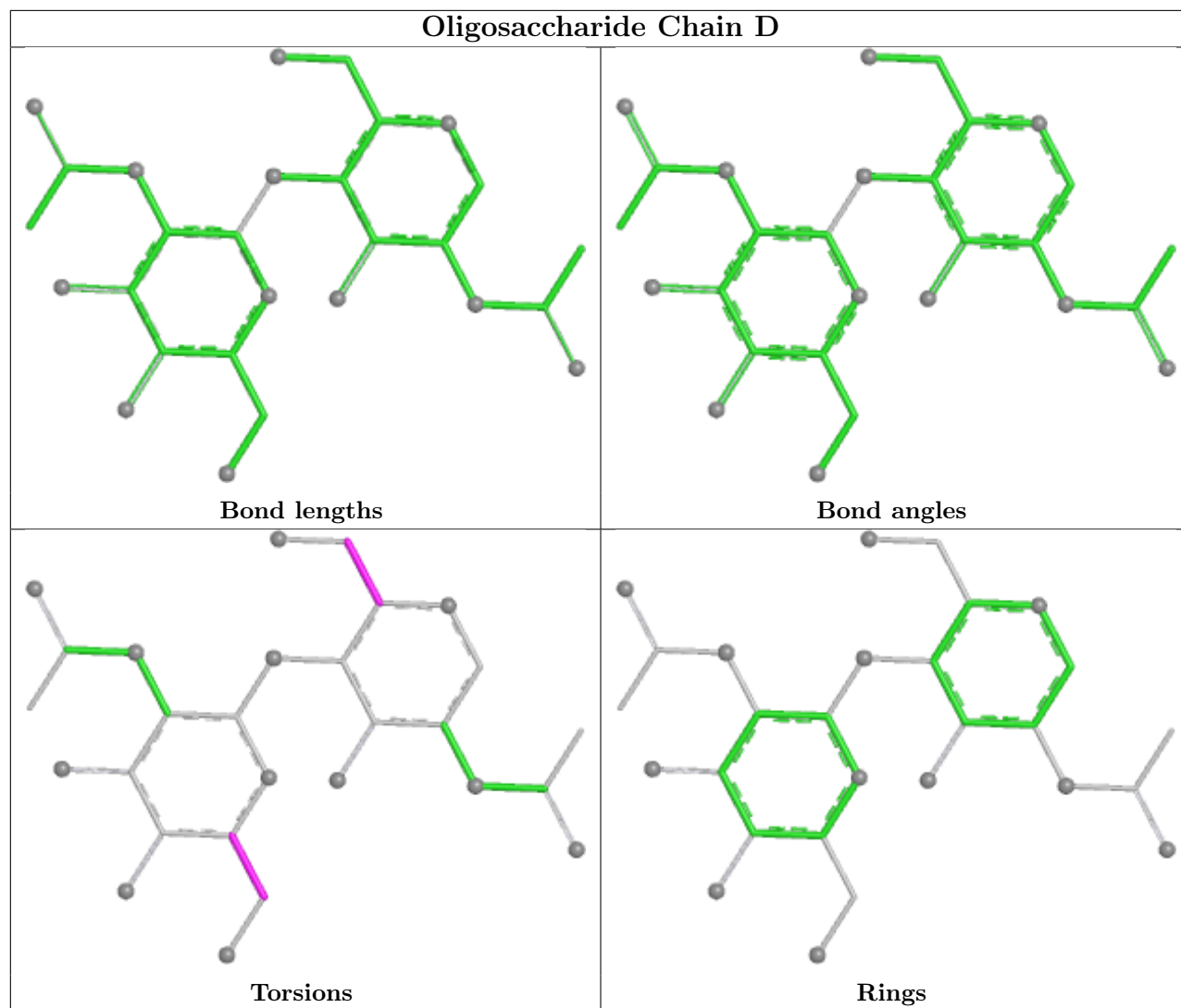
Mol	Chain	Res	Type	Atoms
2	Q	1	NAG	C4-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	K	1	NAG	C4-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6
2	L	1	NAG	C4-C5-C6-O6
2	L	1	NAG	O5-C5-C6-O6
2	L	2	NAG	C4-C5-C6-O6
2	I	2	NAG	C1-C2-N2-C7
2	I	2	NAG	C3-C2-N2-C7
2	K	1	NAG	O5-C5-C6-O6

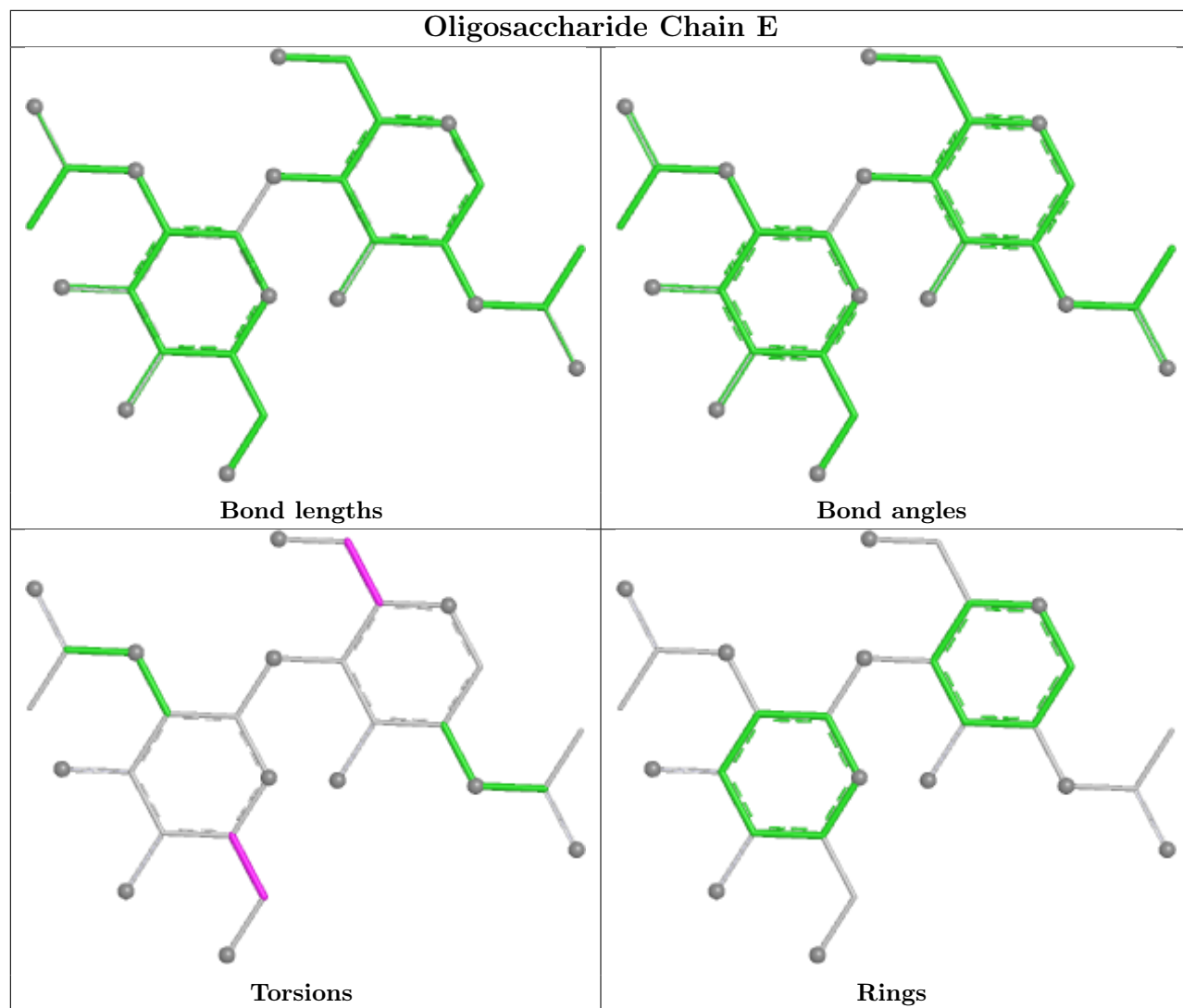
There are no ring outliers.

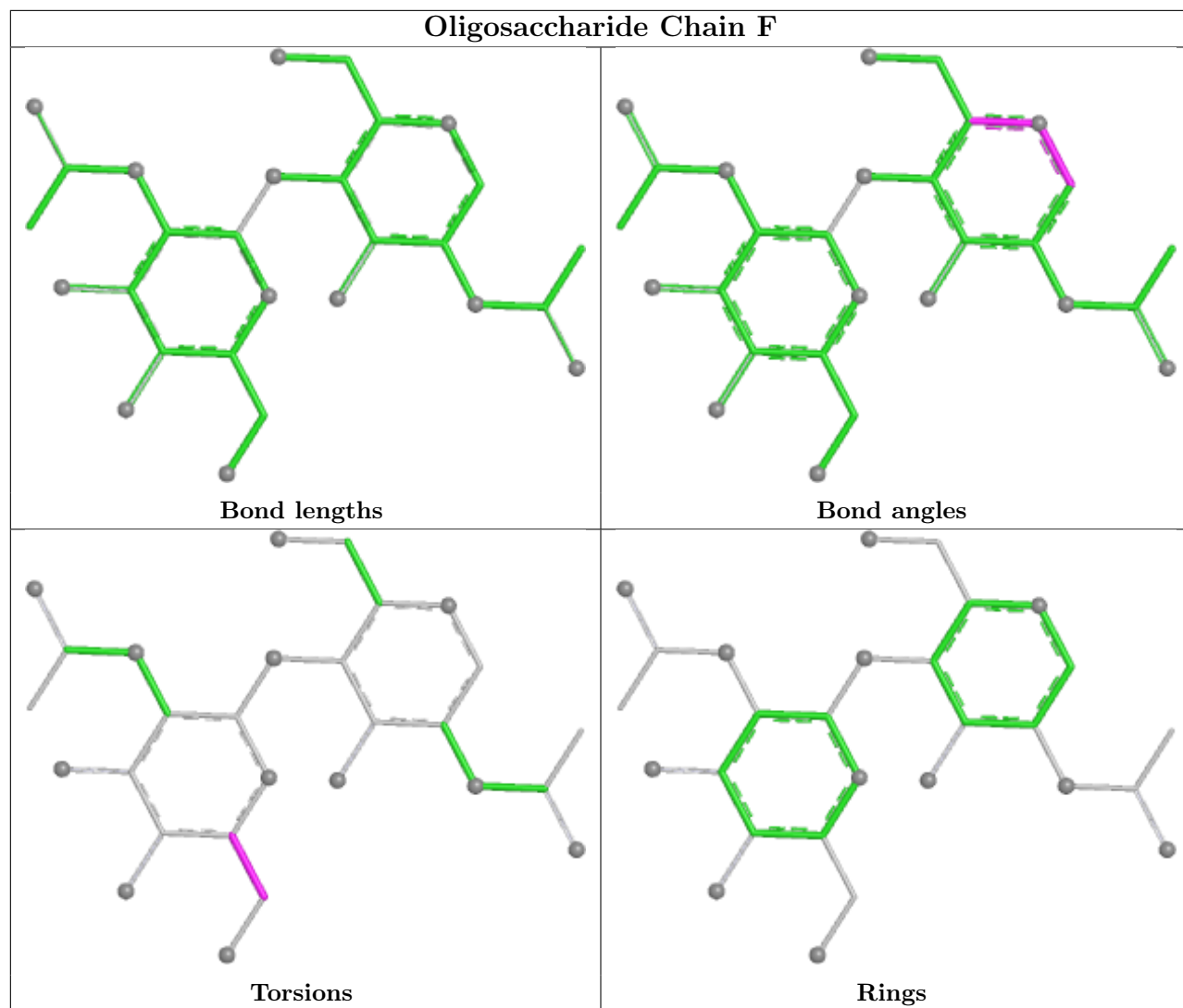
2 monomers are involved in 2 short contacts:

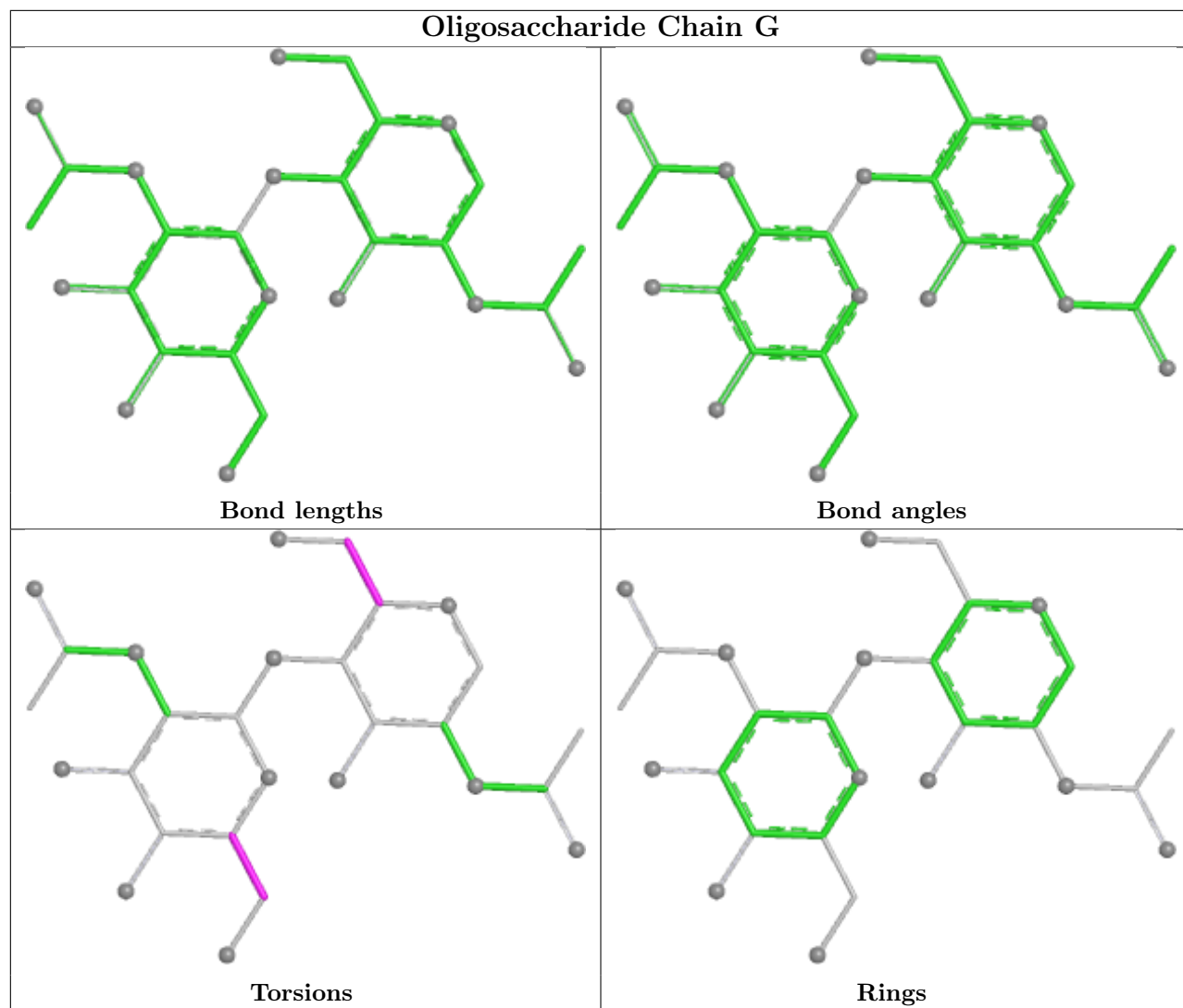
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	P	1	NAG	1	0
2	O	1	NAG	1	0

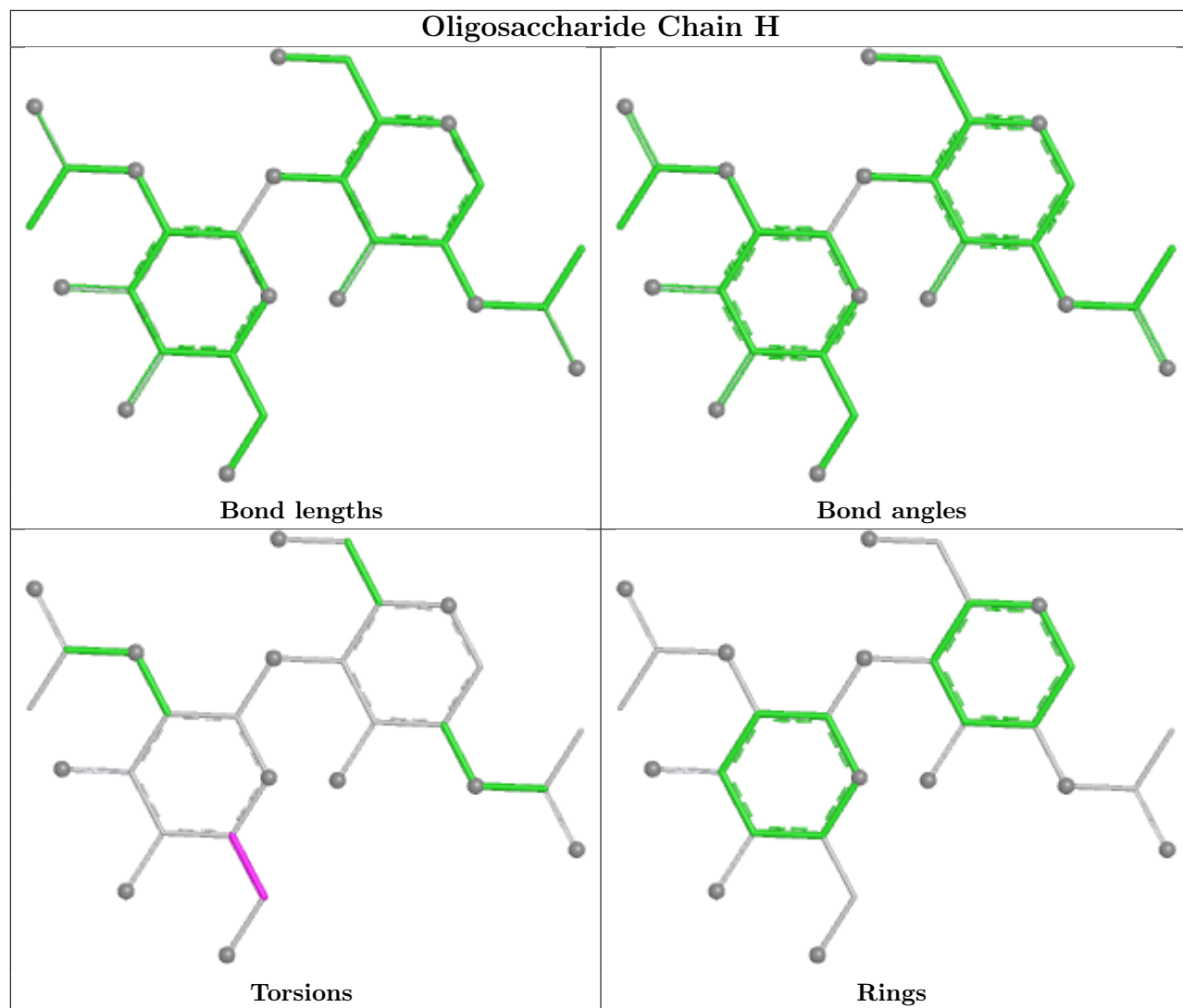
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

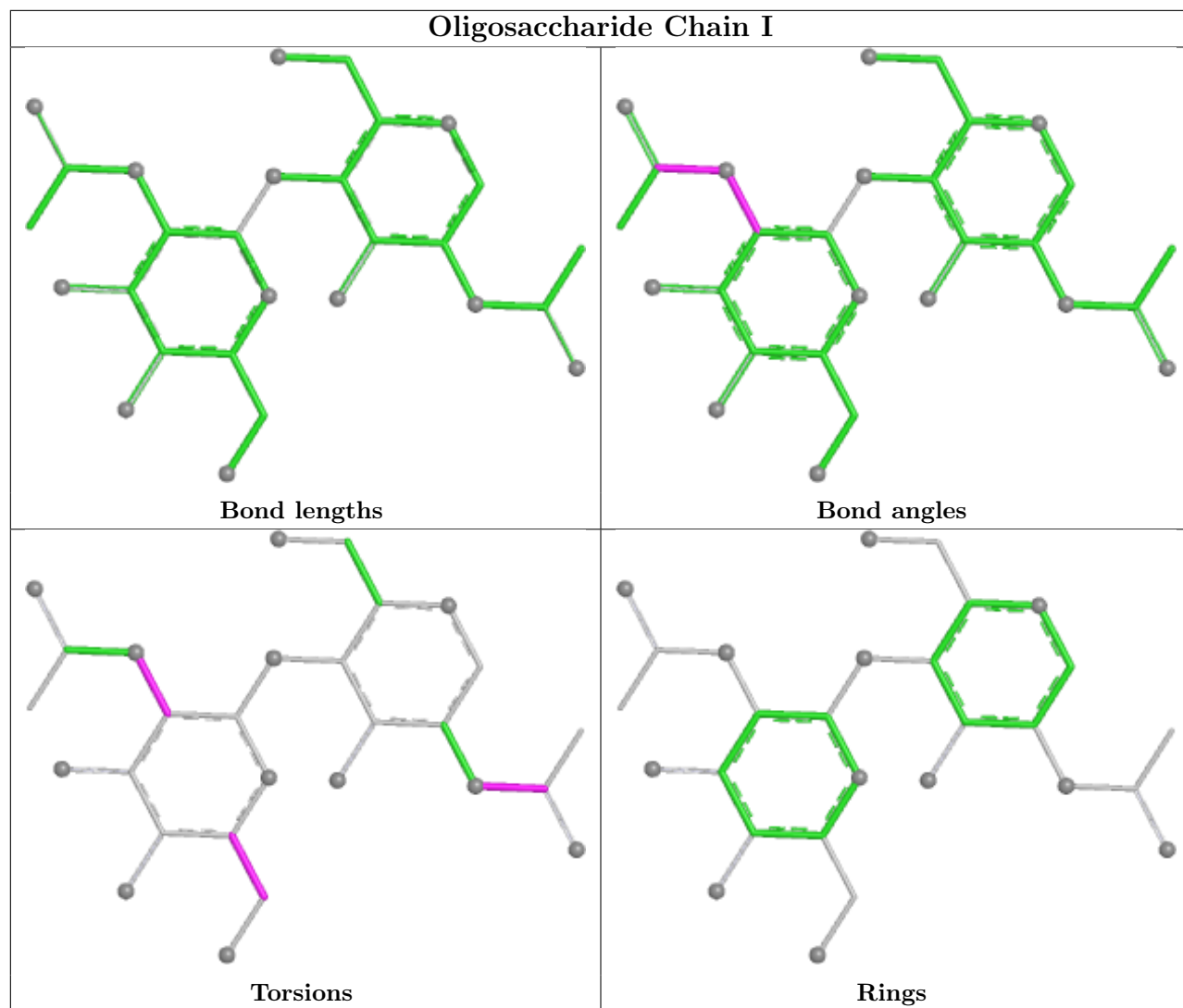


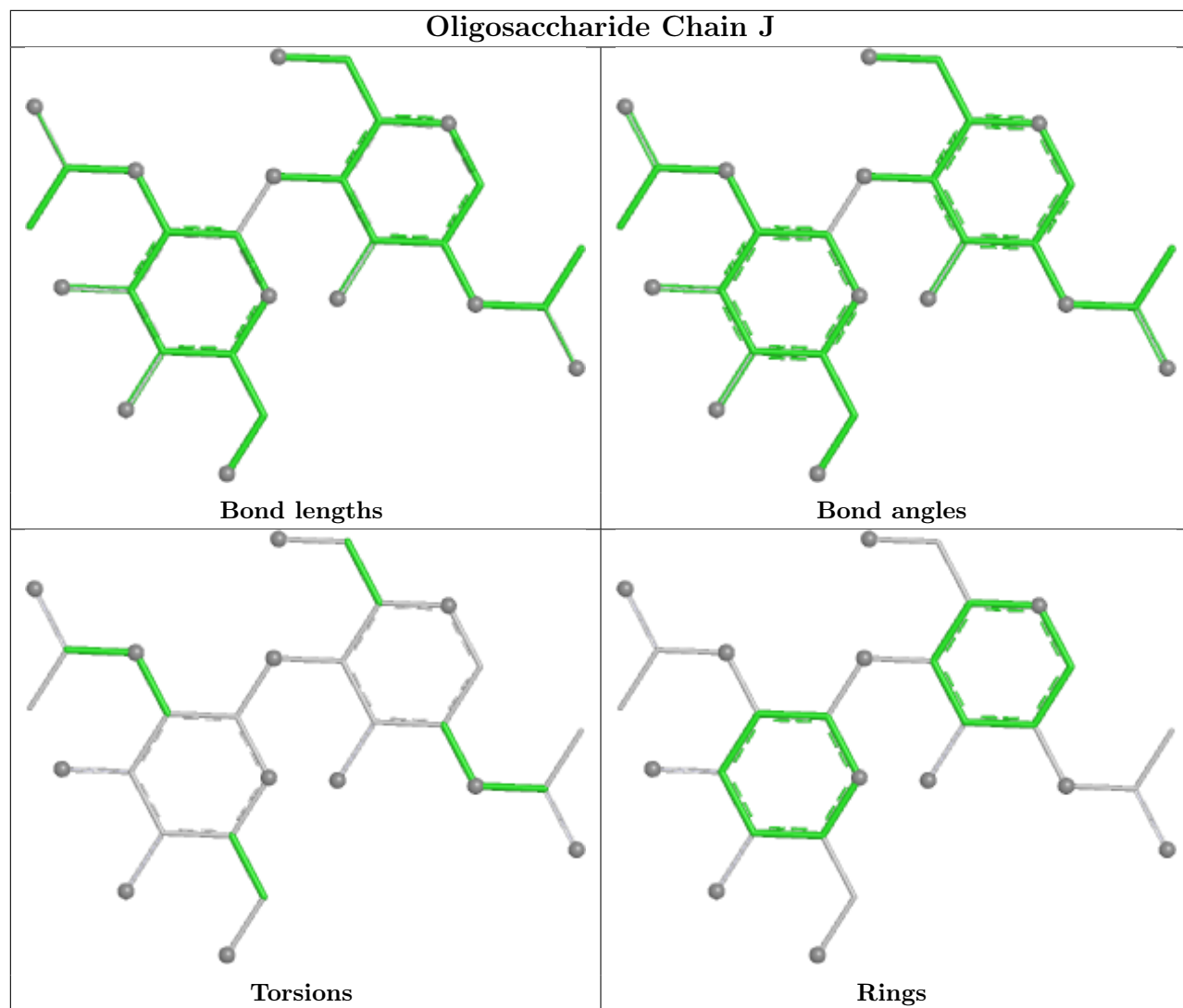


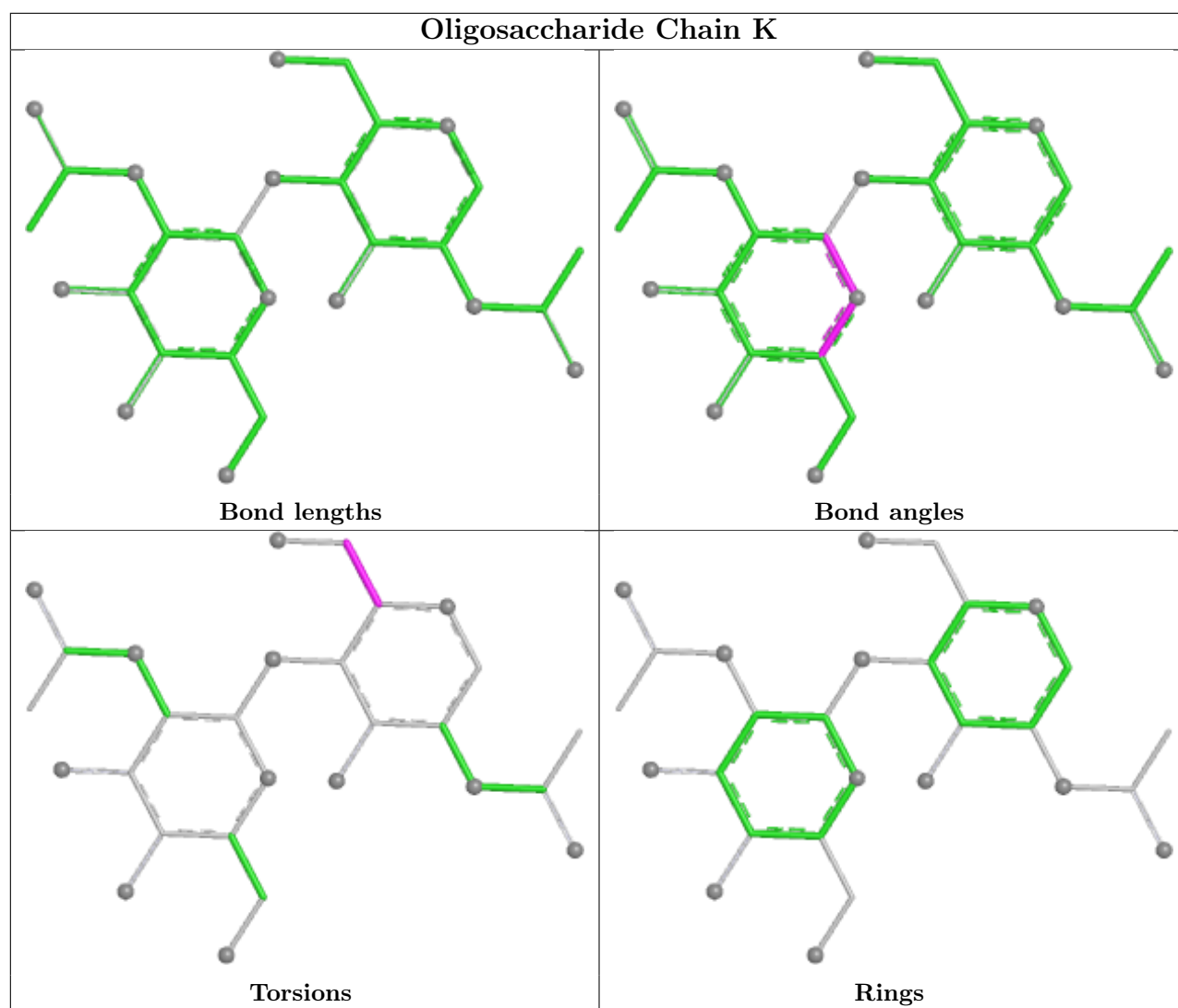


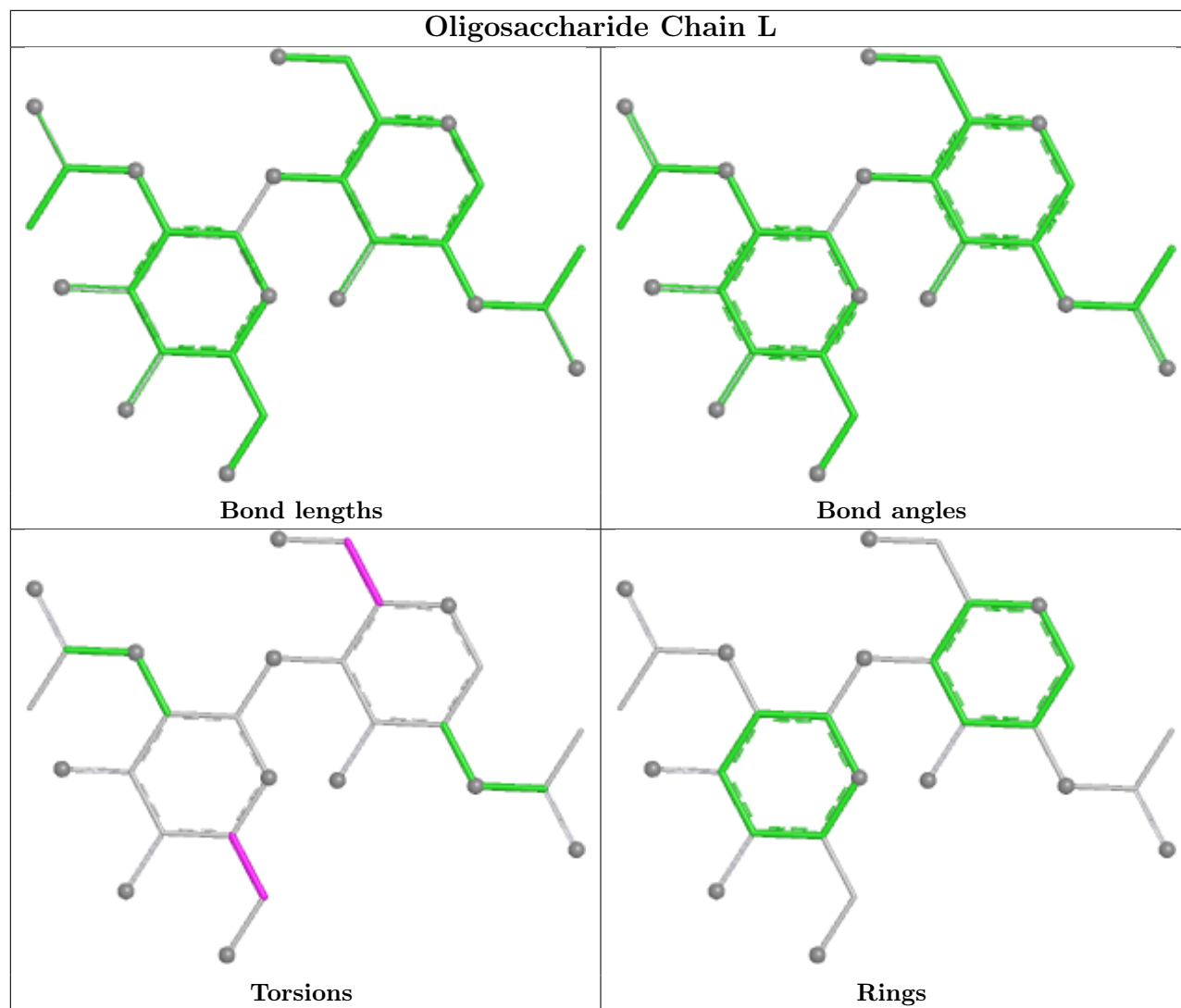


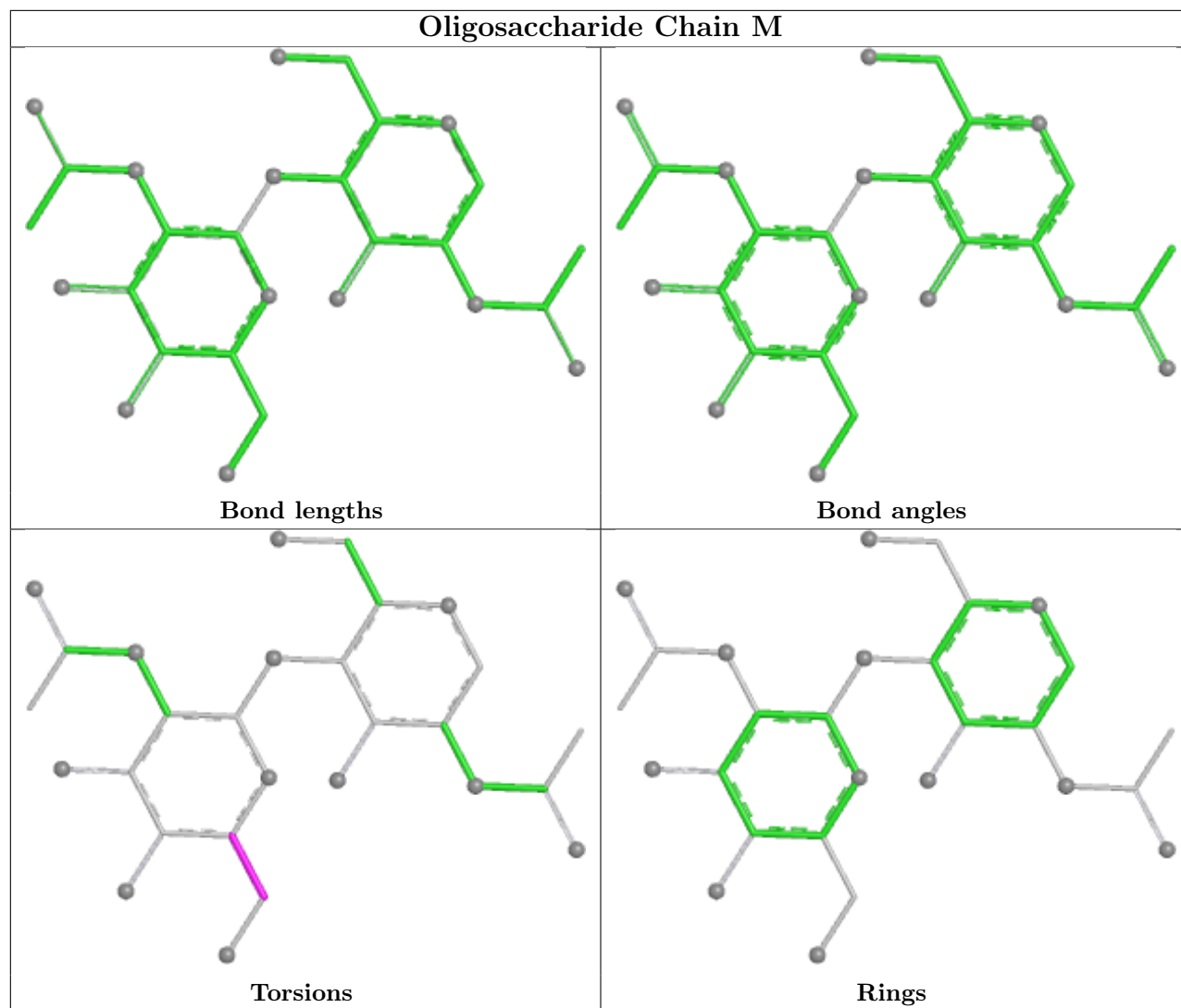


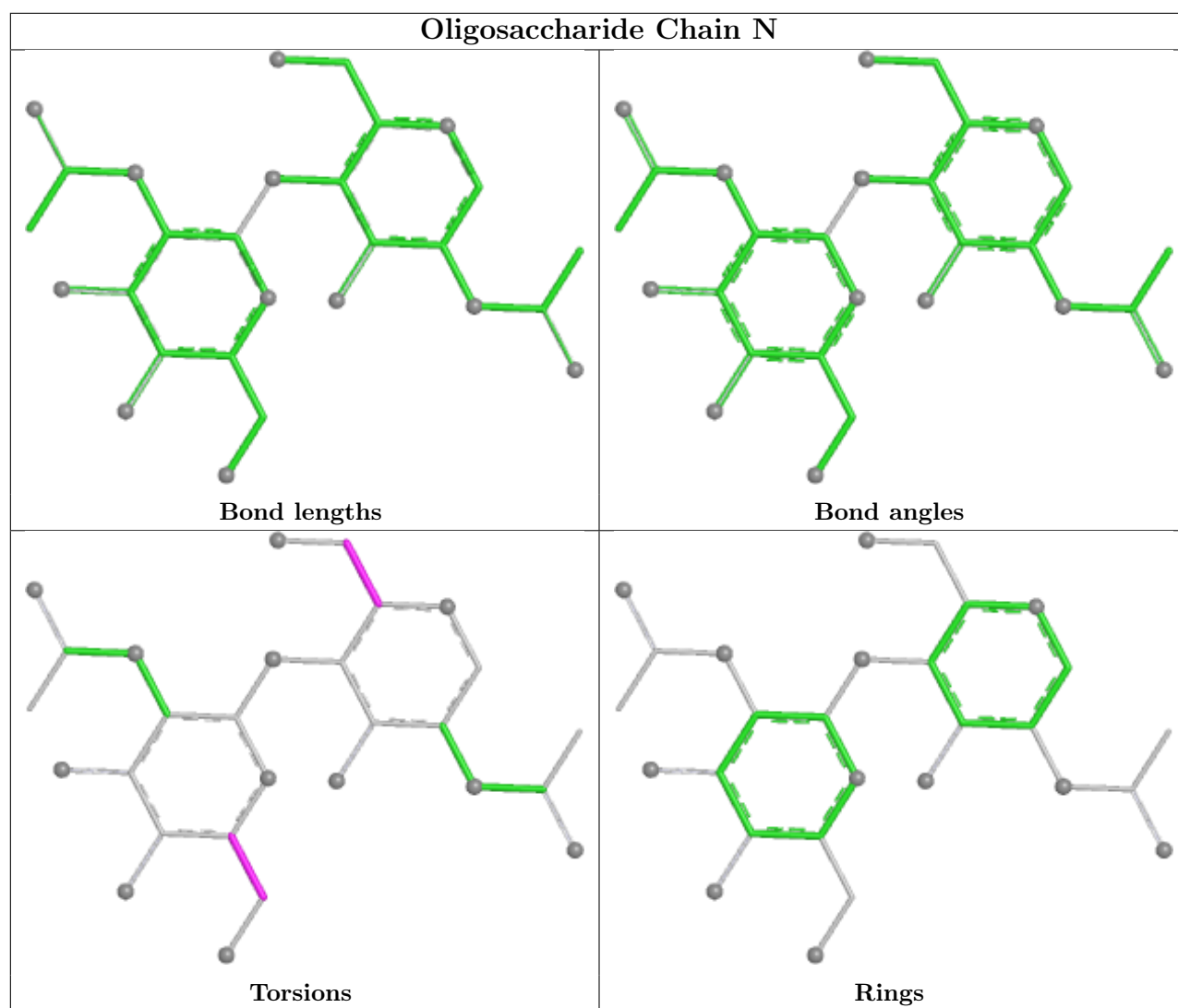


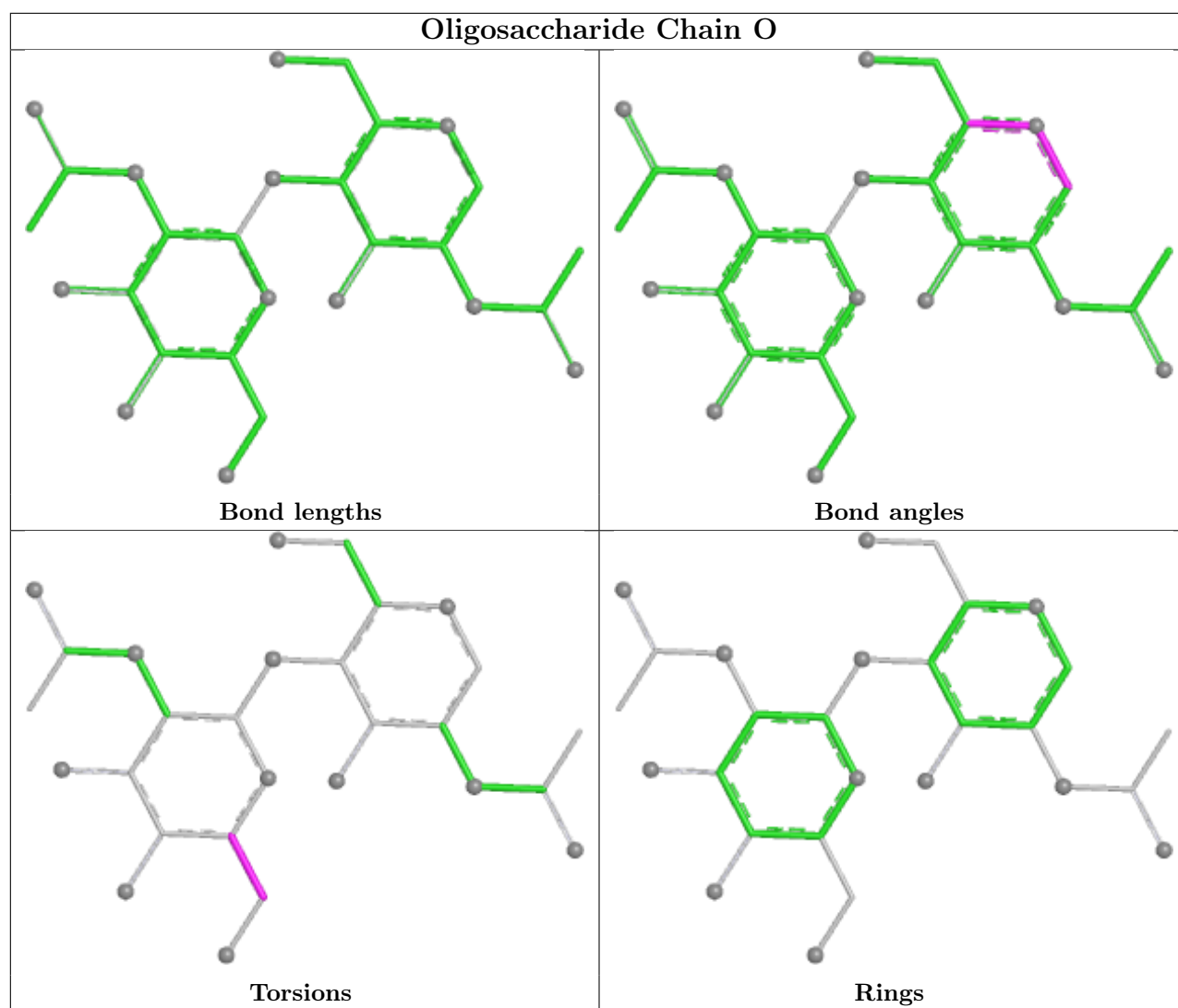


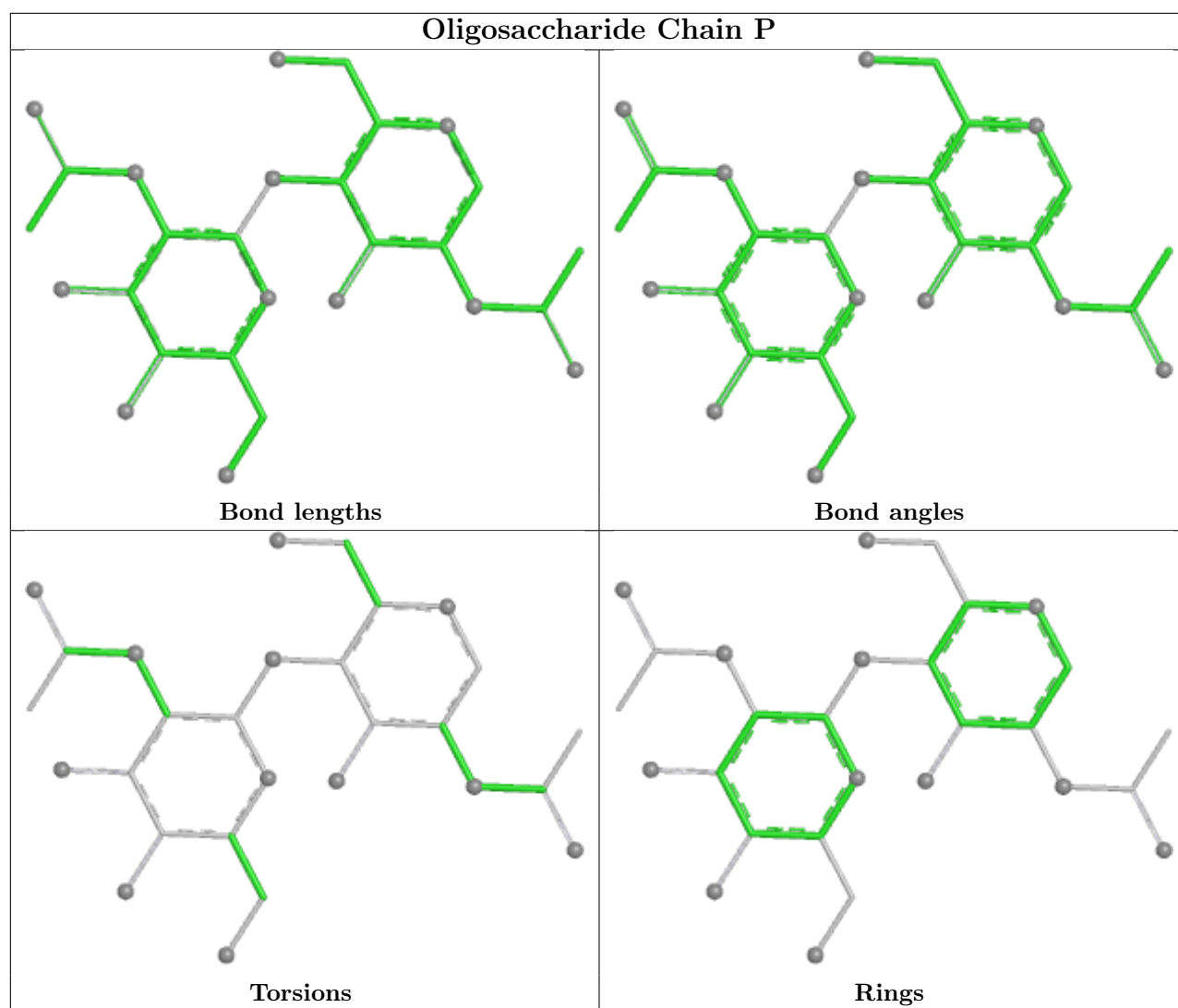


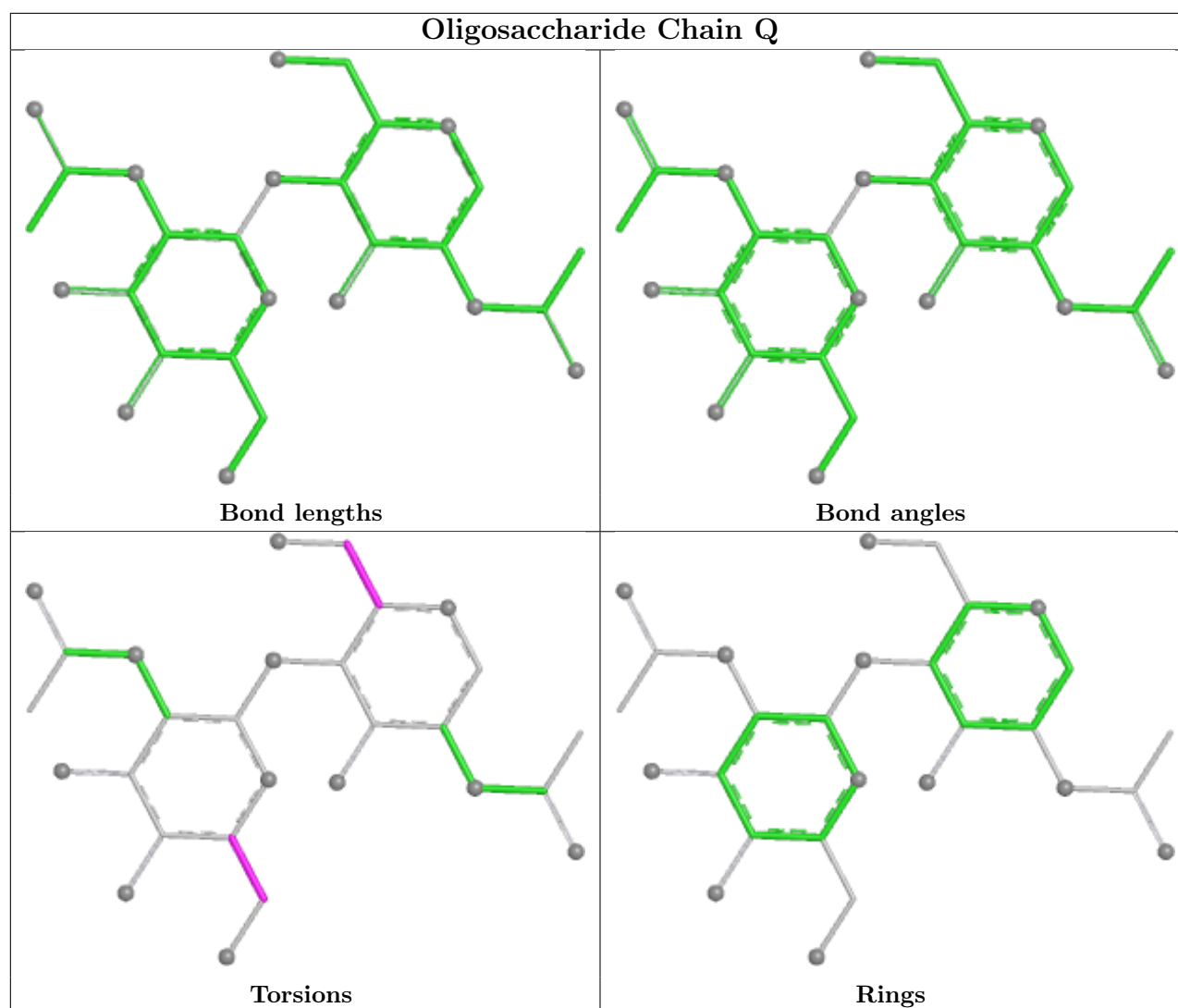












5.6 Ligand geometry [i](#)

14 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	$\# Z > 2$
3	NAG	C	1301	1	14,14,15	1.02	1 (7%)	17,19,21	2.38	4 (23%)
3	NAG	A	1303	1	14,14,15	0.46	0	17,19,21	0.64	1 (5%)
3	NAG	B	1302	1	14,14,15	0.53	0	17,19,21	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	B	1305	1	14,14,15	0.38	0	17,19,21	0.51	0
3	NAG	A	1302	1	14,14,15	0.31	0	17,19,21	0.45	0
3	NAG	B	1306	1	14,14,15	0.50	0	17,19,21	0.63	1 (5%)
3	NAG	C	1302	1	14,14,15	0.30	0	17,19,21	0.62	0
3	NAG	C	1304	1	14,14,15	0.42	0	17,19,21	0.61	1 (5%)
3	NAG	B	1304	1	14,14,15	0.39	0	17,19,21	0.54	0
3	NAG	B	1301	1	14,14,15	1.10	1 (7%)	17,19,21	2.36	4 (23%)
3	NAG	C	1303	1	14,14,15	0.40	0	17,19,21	0.43	0
3	NAG	A	1301	1	14,14,15	0.28	0	17,19,21	0.50	0
3	NAG	B	1303	1	14,14,15	0.45	0	17,19,21	0.65	0
3	NAG	A	1304	1	14,14,15	0.33	0	17,19,21	0.47	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	C	1301	1	-	6/6/23/26	0/1/1/1
3	NAG	A	1303	1	-	3/6/23/26	0/1/1/1
3	NAG	B	1302	1	-	1/6/23/26	0/1/1/1
3	NAG	B	1305	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1302	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1306	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1302	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1304	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1304	1	-	4/6/23/26	0/1/1/1
3	NAG	B	1301	1	-	6/6/23/26	0/1/1/1
3	NAG	C	1303	1	-	1/6/23/26	0/1/1/1
3	NAG	A	1301	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1303	1	-	4/6/23/26	0/1/1/1
3	NAG	A	1304	1	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1301	NAG	C1-C2	3.41	1.57	1.52
3	C	1301	NAG	C1-C2	3.12	1.56	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1301	NAG	C2-N2-C7	8.19	133.88	122.90
3	B	1301	NAG	C2-N2-C7	8.17	133.85	122.90
3	C	1301	NAG	C1-C2-N2	3.98	116.70	110.43
3	B	1301	NAG	C1-C2-N2	3.90	116.58	110.43
3	A	1303	NAG	C1-O5-C5	2.26	115.22	112.19
3	B	1301	NAG	C1-O5-C5	2.19	115.13	112.19
3	B	1306	NAG	C1-O5-C5	2.19	115.12	112.19
3	C	1301	NAG	C8-C7-N2	2.17	119.71	116.12
3	C	1301	NAG	C1-O5-C5	2.14	115.06	112.19
3	B	1301	NAG	C8-C7-N2	2.12	119.63	116.12
3	C	1304	NAG	C1-O5-C5	2.11	115.01	112.19

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1304	NAG	C4-C5-C6-O6
3	C	1301	NAG	O5-C5-C6-O6
3	B	1304	NAG	O5-C5-C6-O6
3	B	1303	NAG	O5-C5-C6-O6
3	A	1302	NAG	O5-C5-C6-O6
3	B	1306	NAG	O5-C5-C6-O6
3	C	1301	NAG	C4-C5-C6-O6
3	A	1301	NAG	O5-C5-C6-O6
3	A	1302	NAG	C4-C5-C6-O6
3	B	1303	NAG	C4-C5-C6-O6
3	B	1301	NAG	O5-C5-C6-O6
3	B	1306	NAG	C4-C5-C6-O6
3	B	1301	NAG	C8-C7-N2-C2
3	B	1301	NAG	O7-C7-N2-C2
3	B	1303	NAG	C8-C7-N2-C2
3	B	1303	NAG	O7-C7-N2-C2
3	B	1304	NAG	C8-C7-N2-C2
3	B	1304	NAG	O7-C7-N2-C2
3	C	1301	NAG	C8-C7-N2-C2
3	C	1301	NAG	O7-C7-N2-C2
3	C	1302	NAG	C8-C7-N2-C2
3	C	1302	NAG	O7-C7-N2-C2
3	A	1301	NAG	C4-C5-C6-O6
3	B	1301	NAG	C4-C5-C6-O6
3	A	1303	NAG	C4-C5-C6-O6
3	A	1303	NAG	O5-C5-C6-O6
3	B	1302	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	C	1303	NAG	O5-C5-C6-O6
3	A	1303	NAG	C1-C2-N2-C7
3	B	1301	NAG	C1-C2-N2-C7
3	C	1301	NAG	C1-C2-N2-C7
3	B	1301	NAG	C3-C2-N2-C7
3	C	1301	NAG	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

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.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-23984. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis ⓘ

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.