



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 12:13 AM UTC

PDB ID : 8BON / pdb_00008bon
EMDB ID : EMD-16144
Title : Structure of the SARS-CoV-2 spike glycoprotein in complex with the macrocyclic peptide S1B3inL1
Authors : Hurdiss, D.L.
Deposited on : 2022-11-15
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

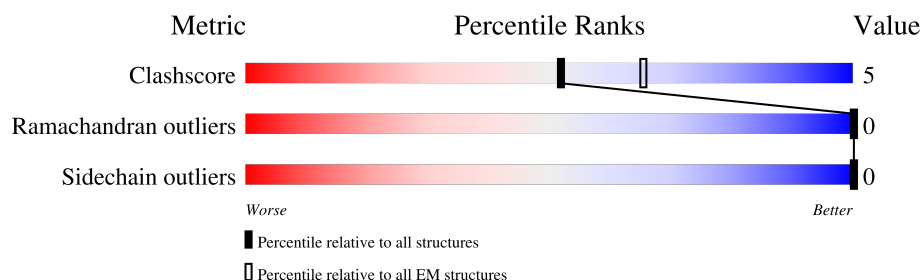
1 Overall quality at a glance

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	1275	71% 13% 16%
1	B	1275	74% 10% 16%
1	C	1275	70% 13% 17%
2	D	19	89% 11%
2	E	19	79% 21%
2	F	19	89% 11%
3	G	2	100%
3	H	2	100%
3	I	2	100%

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

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 25930 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,Fibritin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	1070	Total	C	N	O	S	0	0
			8304	5299	1387	1580	38		
1	A	1069	Total	C	N	O	S	1	0
			8298	5299	1387	1574	38		
1	C	1053	Total	C	N	O	S	0	0
			8168	5210	1364	1556	38		

There are 186 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	682	ALA	ARG	variant	UNP P0DTC2
B	683	ALA	ARG	variant	UNP P0DTC2
B	817	PRO	PHE	variant	UNP P0DTC2
B	892	PRO	ALA	variant	UNP P0DTC2
B	899	PRO	ALA	variant	UNP P0DTC2
B	942	PRO	ALA	variant	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	1209	GLY	-	linker	UNP P0DTC2
B	1210	SER	-	linker	UNP P0DTC2
B	1232	LEU	PHE	engineered mutation	UNP P10104
B	1238	GLY	-	expression tag	UNP P10104
B	1239	ARG	-	expression tag	UNP P10104
B	1240	SER	-	expression tag	UNP P10104
B	1241	LEU	-	expression tag	UNP P10104
B	1242	GLU	-	expression tag	UNP P10104
B	1243	VAL	-	expression tag	UNP P10104
B	1244	LEU	-	expression tag	UNP P10104
B	1245	PHE	-	expression tag	UNP P10104
B	1246	GLN	-	expression tag	UNP P10104
B	1247	GLY	-	expression tag	UNP P10104
B	1248	PRO	-	expression tag	UNP P10104
B	1249	GLY	-	expression tag	UNP P10104
B	1250	HIS	-	expression tag	UNP P10104

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1251	HIS	-	expression tag	UNP P10104
B	1252	HIS	-	expression tag	UNP P10104
B	1253	HIS	-	expression tag	UNP P10104
B	1254	HIS	-	expression tag	UNP P10104
B	1255	HIS	-	expression tag	UNP P10104
B	1256	HIS	-	expression tag	UNP P10104
B	1257	HIS	-	expression tag	UNP P10104
B	1258	SER	-	expression tag	UNP P10104
B	1259	ALA	-	expression tag	UNP P10104
B	1260	TRP	-	expression tag	UNP P10104
B	1261	SER	-	expression tag	UNP P10104
B	1262	HIS	-	expression tag	UNP P10104
B	1263	PRO	-	expression tag	UNP P10104
B	1264	GLN	-	expression tag	UNP P10104
B	1265	PHE	-	expression tag	UNP P10104
B	1266	GLU	-	expression tag	UNP P10104
B	1267	LYS	-	expression tag	UNP P10104
B	1268	GLY	-	expression tag	UNP P10104
B	1269	GLY	-	expression tag	UNP P10104
B	1270	GLY	-	expression tag	UNP P10104
B	1271	SER	-	expression tag	UNP P10104
B	1272	GLY	-	expression tag	UNP P10104
B	1273	GLY	-	expression tag	UNP P10104
B	1274	GLY	-	expression tag	UNP P10104
B	1275	GLY	-	expression tag	UNP P10104
B	1276	SER	-	expression tag	UNP P10104
B	1277	GLY	-	expression tag	UNP P10104
B	1278	GLY	-	expression tag	UNP P10104
B	1279	SER	-	expression tag	UNP P10104
B	1280	ALA	-	expression tag	UNP P10104
B	1281	TRP	-	expression tag	UNP P10104
B	1282	SER	-	expression tag	UNP P10104
B	1283	HIS	-	expression tag	UNP P10104
B	1284	PRO	-	expression tag	UNP P10104
B	1285	GLN	-	expression tag	UNP P10104
B	1286	PHE	-	expression tag	UNP P10104
B	1287	GLU	-	expression tag	UNP P10104
B	1288	LYS	-	expression tag	UNP P10104
A	682	ALA	ARG	variant	UNP P0DTC2
A	683	ALA	ARG	variant	UNP P0DTC2
A	817	PRO	PHE	variant	UNP P0DTC2
A	892	PRO	ALA	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	899	PRO	ALA	variant	UNP P0DTC2
A	942	PRO	ALA	variant	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
A	1209	GLY	-	linker	UNP P0DTC2
A	1210	SER	-	linker	UNP P0DTC2
A	1232	LEU	PHE	engineered mutation	UNP P10104
A	1238	GLY	-	expression tag	UNP P10104
A	1239	ARG	-	expression tag	UNP P10104
A	1240	SER	-	expression tag	UNP P10104
A	1241	LEU	-	expression tag	UNP P10104
A	1242	GLU	-	expression tag	UNP P10104
A	1243	VAL	-	expression tag	UNP P10104
A	1244	LEU	-	expression tag	UNP P10104
A	1245	PHE	-	expression tag	UNP P10104
A	1246	GLN	-	expression tag	UNP P10104
A	1247	GLY	-	expression tag	UNP P10104
A	1248	PRO	-	expression tag	UNP P10104
A	1249	GLY	-	expression tag	UNP P10104
A	1250	HIS	-	expression tag	UNP P10104
A	1251	HIS	-	expression tag	UNP P10104
A	1252	HIS	-	expression tag	UNP P10104
A	1253	HIS	-	expression tag	UNP P10104
A	1254	HIS	-	expression tag	UNP P10104
A	1255	HIS	-	expression tag	UNP P10104
A	1256	HIS	-	expression tag	UNP P10104
A	1257	HIS	-	expression tag	UNP P10104
A	1258	SER	-	expression tag	UNP P10104
A	1259	ALA	-	expression tag	UNP P10104
A	1260	TRP	-	expression tag	UNP P10104
A	1261	SER	-	expression tag	UNP P10104
A	1262	HIS	-	expression tag	UNP P10104
A	1263	PRO	-	expression tag	UNP P10104
A	1264	GLN	-	expression tag	UNP P10104
A	1265	PHE	-	expression tag	UNP P10104
A	1266	GLU	-	expression tag	UNP P10104
A	1267	LYS	-	expression tag	UNP P10104
A	1268	GLY	-	expression tag	UNP P10104
A	1269	GLY	-	expression tag	UNP P10104
A	1270	GLY	-	expression tag	UNP P10104
A	1271	SER	-	expression tag	UNP P10104
A	1272	GLY	-	expression tag	UNP P10104

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1273	GLY	-	expression tag	UNP P10104
A	1274	GLY	-	expression tag	UNP P10104
A	1275	GLY	-	expression tag	UNP P10104
A	1276	SER	-	expression tag	UNP P10104
A	1277	GLY	-	expression tag	UNP P10104
A	1278	GLY	-	expression tag	UNP P10104
A	1279	SER	-	expression tag	UNP P10104
A	1280	ALA	-	expression tag	UNP P10104
A	1281	TRP	-	expression tag	UNP P10104
A	1282	SER	-	expression tag	UNP P10104
A	1283	HIS	-	expression tag	UNP P10104
A	1284	PRO	-	expression tag	UNP P10104
A	1285	GLN	-	expression tag	UNP P10104
A	1286	PHE	-	expression tag	UNP P10104
A	1287	GLU	-	expression tag	UNP P10104
A	1288	LYS	-	expression tag	UNP P10104
C	682	ALA	ARG	variant	UNP P0DTC2
C	683	ALA	ARG	variant	UNP P0DTC2
C	817	PRO	PHE	variant	UNP P0DTC2
C	892	PRO	ALA	variant	UNP P0DTC2
C	899	PRO	ALA	variant	UNP P0DTC2
C	942	PRO	ALA	variant	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	1209	GLY	-	linker	UNP P0DTC2
C	1210	SER	-	linker	UNP P0DTC2
C	1232	LEU	PHE	engineered mutation	UNP P10104
C	1238	GLY	-	expression tag	UNP P10104
C	1239	ARG	-	expression tag	UNP P10104
C	1240	SER	-	expression tag	UNP P10104
C	1241	LEU	-	expression tag	UNP P10104
C	1242	GLU	-	expression tag	UNP P10104
C	1243	VAL	-	expression tag	UNP P10104
C	1244	LEU	-	expression tag	UNP P10104
C	1245	PHE	-	expression tag	UNP P10104
C	1246	GLN	-	expression tag	UNP P10104
C	1247	GLY	-	expression tag	UNP P10104
C	1248	PRO	-	expression tag	UNP P10104
C	1249	GLY	-	expression tag	UNP P10104
C	1250	HIS	-	expression tag	UNP P10104
C	1251	HIS	-	expression tag	UNP P10104
C	1252	HIS	-	expression tag	UNP P10104

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1253	HIS	-	expression tag	UNP P10104
C	1254	HIS	-	expression tag	UNP P10104
C	1255	HIS	-	expression tag	UNP P10104
C	1256	HIS	-	expression tag	UNP P10104
C	1257	HIS	-	expression tag	UNP P10104
C	1258	SER	-	expression tag	UNP P10104
C	1259	ALA	-	expression tag	UNP P10104
C	1260	TRP	-	expression tag	UNP P10104
C	1261	SER	-	expression tag	UNP P10104
C	1262	HIS	-	expression tag	UNP P10104
C	1263	PRO	-	expression tag	UNP P10104
C	1264	GLN	-	expression tag	UNP P10104
C	1265	PHE	-	expression tag	UNP P10104
C	1266	GLU	-	expression tag	UNP P10104
C	1267	LYS	-	expression tag	UNP P10104
C	1268	GLY	-	expression tag	UNP P10104
C	1269	GLY	-	expression tag	UNP P10104
C	1270	GLY	-	expression tag	UNP P10104
C	1271	SER	-	expression tag	UNP P10104
C	1272	GLY	-	expression tag	UNP P10104
C	1273	GLY	-	expression tag	UNP P10104
C	1274	GLY	-	expression tag	UNP P10104
C	1275	GLY	-	expression tag	UNP P10104
C	1276	SER	-	expression tag	UNP P10104
C	1277	GLY	-	expression tag	UNP P10104
C	1278	GLY	-	expression tag	UNP P10104
C	1279	SER	-	expression tag	UNP P10104
C	1280	ALA	-	expression tag	UNP P10104
C	1281	TRP	-	expression tag	UNP P10104
C	1282	SER	-	expression tag	UNP P10104
C	1283	HIS	-	expression tag	UNP P10104
C	1284	PRO	-	expression tag	UNP P10104
C	1285	GLN	-	expression tag	UNP P10104
C	1286	PHE	-	expression tag	UNP P10104
C	1287	GLU	-	expression tag	UNP P10104
C	1288	LYS	-	expression tag	UNP P10104

- Molecule 2 is a protein called Macrocytic peptide S1B3inL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	19	Total	C	N	O	S	0	1
			158	103	30	24	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	19	Total	C	N	O	S	0	1
			158	103	30	24	1		
2	F	19	Total	C	N	O	S	0	1
			158	103	30	24	1		

- 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	G	2	Total	C	N	O	0	0
			28	16	2	10		
3	H	2	Total	C	N	O	0	0
			28	16	2	10		
3	I	2	Total	C	N	O	0	0
			28	16	2	10		
3	J	2	Total	C	N	O	0	0
			28	16	2	10		
3	K	2	Total	C	N	O	0	0
			28	16	2	10		
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		
3	O	2	Total	C	N	O	0	0
			28	16	2	10		
3	P	2	Total	C	N	O	0	0
			28	16	2	10		
3	Q	2	Total	C	N	O	0	0
			28	16	2	10		
3	R	2	Total	C	N	O	0	0
			28	16	2	10		
3	S	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

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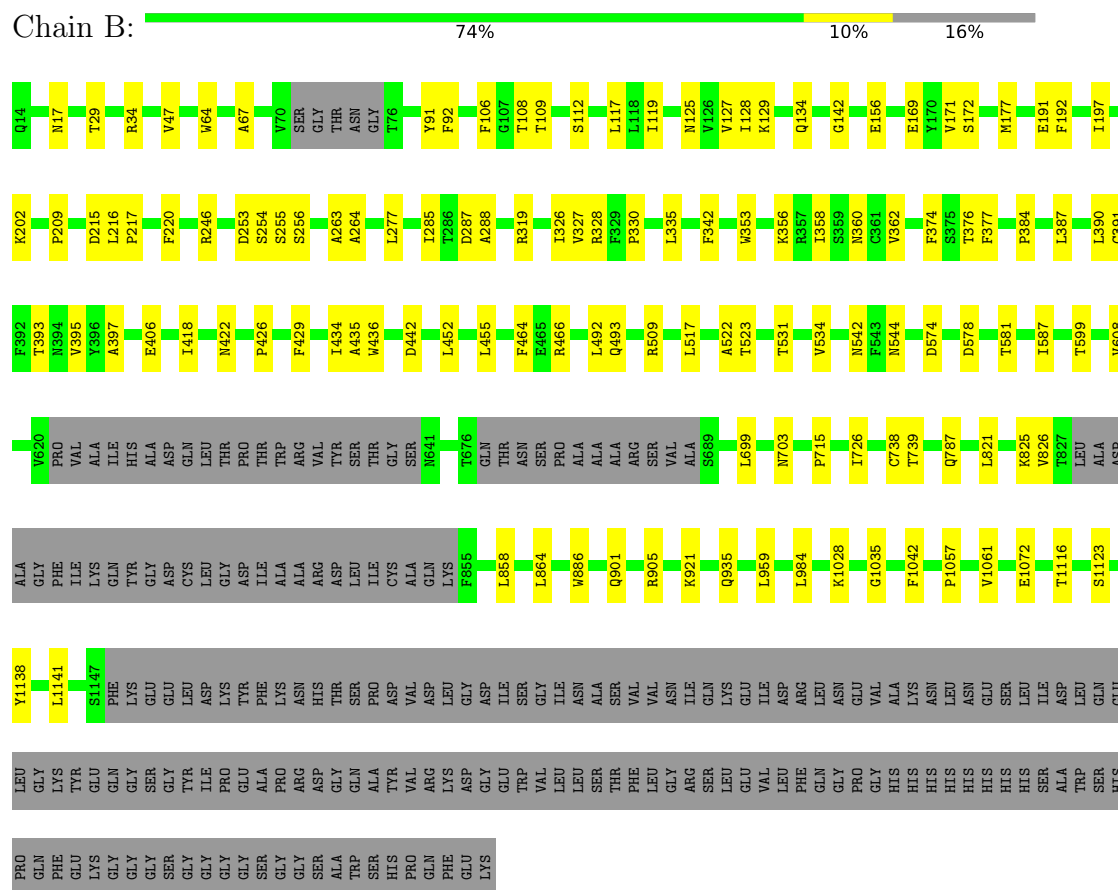
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Mol	Chain	Residues	Atoms				AltConf
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C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

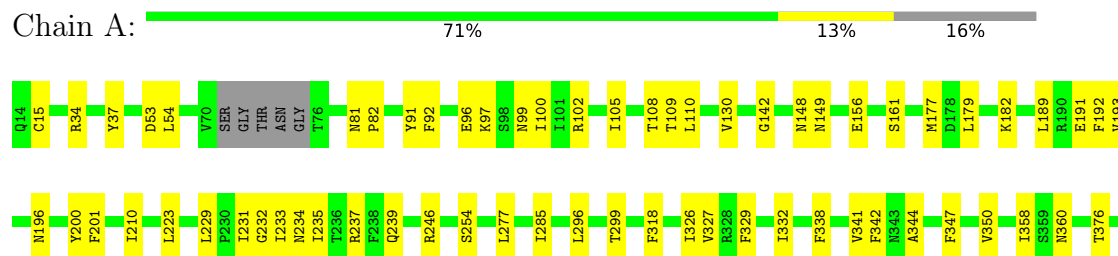
3 Residue-property plots

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,Fibritin



- Molecule 1: Spike glycoprotein,Fibritin



VAL	ARG	LYS	ASP	GLY	GLU	TRP	VAL	LEU	LEU	SER	THR	PHE	LEU	GLY	ARG	SER	LEU	GLN	GLY	PRO	GLY	HIS	HIS	HIS	HIS	HIS	HIS	HIS	SER	ALA	SER	SER	HIS	PRO	GLN	PHE	GLU	LYS	GLY	GLY	GLY	GLY	GLY	GLY	SER	GLY	SER	ALA	TRP	SER
PRO	GLN	PHE	GLU	LYS																																														

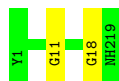
- Molecule 2: Macrocylic peptide S1B3inL1

Chain E:  79% 21%



- Molecule 2: Macrocylic peptide S1B3inL1

Chain D:  89% 11%



- Molecule 2: Macrocylic peptide S1B3inL1

Chain F:  89% 11%

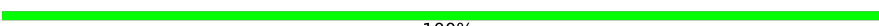


- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  100%

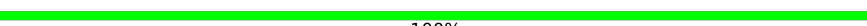


- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  100%



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

Chain I:  100%



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

Chain J:  100%



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

Chain K:  100%



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

Chain L:  50% 50%



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

Chain M:  50% 50%



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

Chain N:  100%



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

Chain O:  100%



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

Chain P:  50% 50%



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

Chain Q:  100%



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

Chain R:  100%



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

Chain S:  100%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	38457	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	49	Depositor
Minimum defocus (nm)	750	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	130000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, CCS, NH2

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	2/8499 (0.0%)	0.32	4/11586 (0.0%)
1	B	0.12	0/8502	0.26	1/11589 (0.0%)
1	C	0.12	0/8360	0.25	0/11388
2	D	0.11	0/151	0.30	0/201
2	E	0.06	0/151	0.16	0/201
2	F	0.06	0/151	0.16	0/201
All	All	0.15	2/25814 (0.0%)	0.28	5/35166 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	384	PRO	CG-CD	-9.17	1.19	1.50
1	A	384	PRO	N-CD	6.70	1.57	1.47

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	384	PRO	CA-N-CD	-13.80	92.68	112.00
1	A	384	PRO	N-CD-CG	-10.67	87.19	103.20
1	A	384	PRO	CA-CB-CG	-6.19	92.74	104.50
1	B	209	PRO	CA-N-CD	-6.17	103.36	112.00
1	A	384	PRO	N-CA-CB	-5.84	97.11	103.25

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	8298	0	8030	111	0
1	B	8304	0	8032	78	0
1	C	8168	0	7890	101	0
2	D	158	0	157	2	0
2	E	158	0	156	3	0
2	F	158	0	157	2	0
3	G	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	1	0
3	M	28	0	25	1	0
3	N	28	0	25	0	0
3	O	28	0	25	0	0
3	P	28	0	25	1	0
3	Q	28	0	25	0	0
3	R	28	0	25	0	0
3	S	28	0	25	0	0
4	A	112	0	103	5	0
4	B	84	0	78	0	0
4	C	126	0	115	1	0
All	All	25930	0	25043	277	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (277) 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:233:ILE:O	4:A:1303:NAG:N2	2.14	0.80
1:A:360:ASN:H	1:A:523:THR:HB	1.51	0.75
1:B:455:LEU:HB2	1:B:493:GLN:HE22	1.54	0.72
1:A:200:TYR:HE1	1:C:521:PRO:HB3	1.56	0.71
1:C:455:LEU:HB2	1:C:493:GLN:HE22	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:804:GLN:NE2	1:A:935:GLN:OE1	2.25	0.70
1:A:656:VAL:HG12	1:A:658:ASN:H	1.57	0.68
1:B:142:GLY:HA3	1:B:156:GLU:HB2	1.76	0.68
1:C:406:GLU:HG2	1:C:418:ILE:HD12	1.77	0.67
1:A:393:THR:HG23	1:A:517:LEU:HD12	1.78	0.66
1:B:358:ILE:HB	1:B:395:VAL:HB	1.79	0.65
1:B:197:ILE:HD11	1:B:202:LYS:HE3	1.80	0.64
1:A:1081:ILE:HD12	1:A:1135:ASN:HB3	1.80	0.63
1:C:825:LYS:HE3	1:C:939:SER:HA	1.80	0.63
1:B:287:ASP:OD1	1:B:288:ALA:N	2.31	0.63
1:B:406:GLU:HG2	1:B:418:ILE:HD12	1.81	0.62
1:B:216:LEU:HD12	1:B:217:PRO:HD2	1.82	0.62
1:B:34:ARG:NH1	1:B:191:GLU:OE2	2.32	0.61
1:B:726:ILE:HG12	1:B:1061:VAL:HG22	1.82	0.61
1:C:229:LEU:HB3	1:C:231:ILE:HG12	1.82	0.61
1:B:177:MET:SD	1:B:177:MET:N	2.73	0.61
1:A:332:ILE:HD11	1:A:525:CYS:HB2	1.83	0.60
1:C:726:ILE:HD13	1:C:945:LEU:HD23	1.83	0.60
1:B:328:ARG:NH1	1:B:531:THR:O	2.34	0.60
1:A:1011:GLN:OE1	1:A:1014:ARG:NH1	2.35	0.60
1:B:356:LYS:HB3	1:B:397:ALA:HB3	1.83	0.59
1:A:177:MET:HG2	1:A:179:LEU:HG	1.85	0.59
1:C:977:LEU:HD11	1:C:993:ILE:HG12	1.84	0.59
1:B:738:CYS:SG	1:B:739:THR:N	2.75	0.58
1:A:108:THR:OG1	1:A:234:ASN:O	2.22	0.58
1:B:327:VAL:HG22	1:B:542:ASN:HB3	1.84	0.58
1:B:377:PHE:HE1	1:B:384:PRO:HB3	1.68	0.58
1:A:108:THR:HG22	1:A:109:THR:HG23	1.85	0.58
1:B:91:TYR:OH	1:B:191:GLU:OE1	2.21	0.58
1:C:21:ARG:NH1	1:C:79:PHE:O	2.36	0.58
2:D:18:GLY:HA3	1:A:466:ARG:H	1.69	0.58
1:C:287:ASP:HB3	1:C:306:PHE:HE2	1.69	0.58
1:A:326:ILE:HG23	1:A:541:PHE:HA	1.86	0.58
1:A:581:THR:HG22	1:A:583:GLU:H	1.69	0.58
1:C:39:PRO:HG3	1:C:51:THR:HG21	1.86	0.57
1:A:409:GLN:HE22	1:A:416:GLY:HA3	1.69	0.57
1:A:1135:ASN:OD1	1:A:1136:THR:N	2.37	0.57
1:C:455:LEU:HB2	1:C:493:GLN:NE2	2.20	0.57
1:B:787:GLN:OE1	1:A:703:ASN:ND2	2.38	0.57
1:B:901:GLN:O	1:B:905:ARG:HG2	2.05	0.57
1:A:766:ALA:HB1	1:A:1012:LEU:HD11	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:902:MET:HG3	1:A:916:LEU:HD11	1.87	0.57
1:A:393:THR:O	1:A:523:THR:OG1	2.21	0.57
1:B:455:LEU:HB2	1:B:493:GLN:NE2	2.20	0.57
4:A:1302:NAG:H3	4:A:1302:NAG:H83	1.87	0.57
1:B:599:THR:HB	1:B:608:VAL:HG12	1.87	0.56
1:B:1116:THR:HG22	1:B:1138:TYR:HB3	1.86	0.56
1:C:147:LYS:O	1:C:150:LYS:NZ	2.38	0.56
1:C:298:GLU:OE2	1:C:316:SER:OG	2.21	0.56
1:A:130:VAL:HG21	1:A:231:ILE:HD12	1.87	0.56
1:A:805:ILE:HD12	1:A:878:LEU:HD11	1.87	0.56
1:B:376:THR:HB	1:B:435:ALA:HB3	1.87	0.56
1:C:393:THR:HG23	1:C:517:LEU:HD12	1.85	0.56
1:B:984:LEU:O	1:A:386:LYS:NZ	2.32	0.56
1:A:426:PRO:HD2	1:A:429:PHE:HB2	1.85	0.56
1:C:374:PHE:HA	1:C:436:TRP:HB3	1.88	0.56
1:B:335:LEU:HD13	1:B:362:VAL:HG13	1.87	0.56
1:C:358:ILE:HB	1:C:395:VAL:HB	1.86	0.56
1:B:67:ALA:O	1:B:263:ALA:N	2.37	0.56
1:B:246:ARG:NH2	1:B:254:SER:O	2.39	0.56
1:A:671:CYS:SG	1:A:697:MET:HE2	2.46	0.56
1:A:15:CYS:SG	1:A:161:SER:OG	2.63	0.55
1:A:342:PHE:HE2	1:A:434:ILE:HG21	1.70	0.55
1:C:125:ASN:ND2	1:C:172:SER:O	2.36	0.55
4:C:1308:NAG:H83	4:C:1308:NAG:H3	1.88	0.55
1:C:326:ILE:HD11	1:C:533:LEU:HA	1.87	0.55
1:B:29:THR:OG1	1:B:215:ASP:OD1	2.25	0.55
1:A:376:THR:HB	1:A:435:ALA:HB3	1.87	0.54
1:A:338:PHE:HA	1:A:341:VAL:HG12	1.89	0.54
1:B:374:PHE:HA	1:B:436:TRP:HB3	1.89	0.54
1:B:119:ILE:HG12	1:B:128:ILE:HG12	1.89	0.54
1:B:864:LEU:HG	1:A:697:MET:HE1	1.90	0.54
1:A:246:ARG:NH2	1:A:254:SER:O	2.40	0.54
1:C:391:CYS:HB3	1:C:522:ALA:HB1	1.90	0.54
1:C:878:LEU:HD21	1:C:1052:PHE:HB3	1.89	0.54
1:A:142:GLY:HA3	1:A:156:GLU:HB2	1.90	0.53
1:A:518:LEU:O	1:A:519:HIS:ND1	2.41	0.53
1:A:327:VAL:H	1:A:531:THR:HG22	1.73	0.53
1:C:577:ARG:HG3	1:C:584:ILE:HG22	1.90	0.53
1:A:930:ALA:O	1:A:934:ILE:HG12	2.09	0.53
1:A:277:LEU:HD12	1:A:285:ILE:HD13	1.91	0.53
1:A:34:ARG:NH1	1:A:191:GLU:OE2	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:MET:SD	1:A:177:MET:N	2.82	0.53
1:A:422:ASN:HD21	1:A:454:ARG:H	1.57	0.52
1:B:426:PRO:HD2	1:B:429:PHE:HB2	1.92	0.52
1:C:130:VAL:HG12	1:C:168:PHE:HB3	1.91	0.52
1:C:376:THR:HB	1:C:435:ALA:HB3	1.91	0.52
1:B:125:ASN:ND2	1:B:172:SER:O	2.39	0.52
1:C:985:ASP:HB3	1:C:987:PRO:HD2	1.92	0.51
1:A:770:ILE:HD11	1:A:1012:LEU:HD12	1.91	0.51
1:A:1102:TRP:HB2	1:A:1135:ASN:ND2	2.26	0.51
1:C:246:ARG:NH2	1:C:254:SER:O	2.44	0.51
1:A:1134:ASN:OD1	3:M:1:NAG:N2	2.43	0.51
1:A:53:ASP:OD1	1:A:54:LEU:N	2.44	0.51
1:C:1083:HIS:O	1:C:1085:GLY:N	2.44	0.51
1:B:17:ASN:O	1:B:255:SER:OG	2.29	0.51
1:A:201:PHE:HB3	1:A:229:LEU:HB2	1.93	0.51
1:B:464:PHE:HB3	2:E:16:PHE:HA	1.93	0.50
1:A:736:VAL:HG11	1:A:1004:LEU:HD11	1.93	0.50
1:C:715:PRO:HA	1:C:1072:GLU:HA	1.93	0.50
1:A:901:GLN:O	1:A:905:ARG:HG2	2.11	0.50
1:A:329:PHE:O	1:A:580:GLN:NE2	2.42	0.50
1:A:404:GLY:HA2	1:A:508:TYR:CD2	2.46	0.50
1:B:821:LEU:HD22	1:B:935:GLN:OE1	2.12	0.50
1:A:231:ILE:HG22	1:A:233:ILE:HG23	1.94	0.49
1:B:47:VAL:HG23	1:A:569:ILE:HG13	1.93	0.49
1:B:277:LEU:HD12	1:B:285:ILE:HD13	1.93	0.49
1:C:231:ILE:HG22	1:C:233:ILE:HG23	1.93	0.49
1:B:715:PRO:HA	1:B:1072:GLU:HA	1.95	0.49
1:B:826:VAL:HG21	1:B:1057:PRO:HG2	1.94	0.49
1:A:973:ILE:HB	1:A:980:ILE:HD13	1.93	0.49
1:B:703:ASN:ND2	1:C:787:GLN:OE1	2.33	0.49
1:A:189:LEU:HB2	1:A:210:ILE:HD13	1.94	0.49
1:A:448:ASN:OD1	1:A:450:ASN:ND2	2.41	0.49
1:C:784:GLN:HG3	1:C:1029:MET:HG2	1.95	0.49
1:C:377:PHE:HE2	1:C:384:PRO:HB3	1.78	0.49
1:B:393:THR:HG23	1:B:517:LEU:HD12	1.95	0.48
1:A:233:ILE:C	4:A:1303:NAG:N2	2.71	0.48
1:A:347:PHE:CE2	1:A:399:SER:HB3	2.48	0.48
1:B:67:ALA:HB3	1:B:263:ALA:HB3	1.95	0.48
1:A:97:LYS:NZ	1:A:182:LYS:O	2.41	0.48
1:C:898:PHE:HA	1:C:901:GLN:HG2	1.96	0.48
1:C:90:VAL:HG21	1:C:238:PHE:CZ	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:102:ARG:HG3	1:C:141:LEU:HD12	1.96	0.48
1:C:749:CYS:SG	1:C:997:ILE:HD11	2.54	0.48
1:A:1082:CYS:HB3	1:A:1132:ILE:HD11	1.96	0.47
1:A:105:ILE:HG13	1:A:239:GLN:HB3	1.95	0.47
1:B:220:PHE:HE2	1:B:285:ILE:HG22	1.80	0.47
1:C:128:ILE:HG21	1:C:229:LEU:HD21	1.95	0.47
2:D:11:GLY:HA2	1:A:430:THR:HG21	1.97	0.47
1:A:452:LEU:HB3	1:A:492:LEU:HD12	1.95	0.47
1:A:616:ASN:OD1	1:A:617:CYS:N	2.48	0.47
1:C:308:VAL:HB	1:C:602:THR:HG23	1.96	0.47
1:C:434:ILE:HB	1:C:511:VAL:HB	1.96	0.47
1:A:344:ALA:HB3	1:A:347:PHE:HE1	1.78	0.47
1:C:100:ILE:HG22	1:C:242:LEU:HD12	1.96	0.47
1:B:442:ASP:OD1	1:B:509:ARG:NH2	2.37	0.47
1:A:1005:GLN:OE1	1:C:1002:GLN:NE2	2.48	0.47
1:B:353:TRP:O	1:B:466:ARG:NE	2.48	0.46
1:A:350:VAL:HG12	1:A:422:ASN:HB3	1.97	0.46
1:C:109:THR:OG1	1:C:111:ASP:OD1	2.31	0.46
1:A:409:GLN:HG2	1:A:419:ALA:HB2	1.96	0.46
1:A:99:ASN:O	1:A:102:ARG:NH2	2.48	0.46
1:B:156:GLU:OE2	1:B:246:ARG:NH1	2.47	0.46
1:A:391:CYS:HB3	1:A:522:ALA:HB1	1.97	0.46
1:A:409:GLN:NE2	1:A:416:GLY:HA3	2.30	0.46
1:C:426:PRO:HD2	1:C:429:PHE:HB2	1.96	0.46
1:A:193:VAL:HG23	1:A:223:LEU:HD12	1.98	0.46
1:B:391:CYS:HB3	1:B:522:ALA:HB1	1.96	0.46
1:A:232:GLY:HA2	4:A:1303:NAG:H82	1.67	0.46
1:A:1028:LYS:NZ	1:A:1042:PHE:O	2.34	0.46
1:A:148:ASN:OD1	1:A:149:ASN:ND2	2.35	0.46
1:C:383:SER:HB3	1:C:386:LYS:HE2	1.98	0.46
1:C:353:TRP:O	1:C:466:ARG:NE	2.49	0.46
1:A:196:ASN:HA	1:A:200:TYR:O	2.16	0.46
1:B:112:SER:HB3	1:B:134:GLN:HB2	1.98	0.45
1:C:452:LEU:HD12	1:C:492:LEU:HB3	1.98	0.45
1:B:1035:GLY:HA3	1:A:1040:VAL:HG21	1.97	0.45
1:A:804:GLN:OE1	3:L:1:NAG:O6	2.33	0.45
1:C:383:SER:HB3	1:C:386:LYS:HB2	1.97	0.45
1:B:858:LEU:HD23	1:B:959:LEU:HD22	1.98	0.45
1:C:387:LEU:H	1:C:387:LEU:HD23	1.82	0.45
1:C:422:ASN:OD1	1:C:454:ARG:N	2.45	0.45
1:B:253:ASP:OD1	1:B:256:SER:OG	2.33	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:736:VAL:HG22	1:A:858:LEU:HD22	1.98	0.45
1:C:142:GLY:HA3	1:C:156:GLU:HB2	1.97	0.45
1:B:1028:LYS:NZ	1:B:1042:PHE:O	2.30	0.45
1:C:80:ASP:OD1	1:C:80:ASP:N	2.44	0.45
1:A:91:TYR:OH	1:A:191:GLU:OE1	2.29	0.45
1:C:555:SER:OG	1:C:584:ILE:HG13	2.16	0.45
1:C:763:LEU:HD22	1:C:1008:VAL:HG21	1.98	0.45
1:A:358:ILE:HB	1:A:395:VAL:HB	1.99	0.45
1:C:645:THR:HG23	1:C:647:ALA:H	1.81	0.45
1:C:294:ASP:OD1	1:C:294:ASP:N	2.50	0.44
1:C:303:LEU:HD12	1:C:308:VAL:HG22	1.98	0.44
1:A:81:ASN:N	1:A:82:PRO:HD3	2.32	0.44
1:B:418:ILE:HA	1:B:422:ASN:HD22	1.83	0.44
1:A:92:PHE:O	1:A:192:PHE:N	2.46	0.44
1:C:18:LEU:HD12	1:C:258:TRP:CE2	2.52	0.44
1:C:327:VAL:HA	1:C:542:ASN:HB3	1.99	0.44
1:C:908:GLY:O	1:C:1038:LYS:NZ	2.50	0.44
1:B:387:LEU:HD23	1:B:387:LEU:H	1.83	0.44
1:C:533:LEU:HD21	1:C:585:LEU:HD11	2.00	0.44
1:A:520:ALA:HB1	1:A:521:PRO:HD2	1.99	0.44
1:C:328:ARG:NH2	1:C:578:ASP:OD2	2.46	0.44
1:A:598:ILE:HG23	1:A:664:ILE:HG21	1.99	0.44
1:C:86:PHE:N	1:C:236:THR:O	2.41	0.44
1:C:115:GLN:HG2	1:C:233:ILE:HG21	1.99	0.44
1:C:517:LEU:HD23	2:F:9:ILE:HB	2.00	0.44
1:C:736:VAL:HG22	1:C:858:LEU:HD22	2.00	0.44
1:C:1101:HIS:ND1	3:P:1:NAG:H5	2.33	0.43
1:C:1125:ASN:ND2	1:C:1127:ASP:OD2	2.50	0.43
1:B:117:LEU:HD21	1:B:119:ILE:HG13	1.99	0.43
1:A:229:LEU:HB3	1:A:231:ILE:HD11	1.99	0.43
1:C:201:PHE:HB3	1:C:229:LEU:HB2	1.99	0.43
1:C:703:ASN:OD1	1:C:704:SER:N	2.51	0.43
1:C:901:GLN:O	1:C:905:ARG:HG2	2.18	0.43
1:C:1090:PRO:HD3	1:C:1095:PHE:CE2	2.53	0.43
1:B:326:ILE:HD13	1:B:534:VAL:HG22	1.99	0.43
1:B:390:LEU:HD12	1:B:390:LEU:HA	1.88	0.43
1:B:1141:LEU:HD13	1:A:1141:LEU:HD11	1.99	0.43
1:C:395:VAL:HG23	1:C:524:VAL:HG21	2.00	0.43
1:A:1035:GLY:HA3	1:C:1040:VAL:HG21	2.01	0.43
1:A:296:LEU:O	1:A:299:THR:OG1	2.34	0.43
1:C:442:ASP:OD1	1:C:509:ARG:NH2	2.40	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:699:LEU:HD21	1:C:869:MET:HG2	2.00	0.43
1:A:904:TYR:CZ	1:C:1107:ARG:HD3	2.53	0.43
1:C:40:ASP:N	1:C:40:ASP:OD1	2.51	0.43
1:A:722:VAL:HG22	1:A:1065:VAL:HG22	2.01	0.42
1:C:498:GLN:N	1:C:501:ASN:OD1	2.49	0.42
1:B:921:LYS:HD2	1:B:921:LYS:HA	1.81	0.42
1:A:318:PHE:HZ	1:A:615:VAL:HG11	1.84	0.42
1:C:30:ASN:HD21	1:C:59:PHE:HD1	1.67	0.42
1:C:65:PHE:HE2	1:C:84:LEU:HD11	1.83	0.42
1:C:792:PRO:O	1:C:795:LYS:NZ	2.40	0.42
1:B:1123:SER:OG	1:C:914:ASN:ND2	2.51	0.42
2:E:7:GLN:HB2	2:E:8:ILE:HD12	2.01	0.42
1:A:763:LEU:HD22	1:A:1008:VAL:HG21	2.01	0.42
1:C:1093:GLY:O	1:C:1107:ARG:NH1	2.52	0.42
1:A:773:GLU:OE2	1:A:1019:ARG:HD3	2.20	0.42
1:A:110:LEU:HG	1:A:237:ARG:HH12	1.84	0.42
1:A:986:PRO:N	1:A:987:PRO:HD2	2.34	0.42
1:A:976:VAL:HG12	1:A:979:ASP:H	1.84	0.42
1:A:1019:ARG:HH22	1:C:1017:GLU:HG2	1.83	0.42
1:C:273:ARG:HH21	1:C:292:ALA:HB3	1.84	0.42
1:A:342:PHE:CE2	1:A:434:ILE:HG21	2.51	0.42
1:A:403:ARG:HH21	1:A:405:ASP:HB2	1.85	0.42
1:C:719:THR:HG23	1:C:1070:ALA:HB2	2.01	0.42
1:B:574:ASP:O	1:B:587:ILE:N	2.49	0.42
1:C:320:VAL:HG23	1:C:590:CYS:HB3	2.01	0.42
1:C:426:PRO:HB3	2:F:14:TRP:CD1	2.54	0.42
1:A:92:PHE:HB3	1:A:192:PHE:HB2	2.02	0.42
1:A:383:SER:HB3	1:A:386:LYS:HB3	2.02	0.42
1:A:869:MET:HE1	1:C:697:MET:HG3	2.01	0.42
1:B:64:TRP:HE1	1:B:264:ALA:HB1	1.85	0.42
1:B:452:LEU:HD12	1:B:492:LEU:HB3	2.02	0.42
1:B:517:LEU:HD23	2:E:9:ILE:HB	2.02	0.42
1:C:69:HIS:C	1:C:77:LYS:H	2.28	0.42
1:B:92:PHE:O	1:B:192:PHE:N	2.38	0.41
1:B:330:PRO:HG3	1:B:544:ASN:HD21	1.84	0.41
1:C:32:PHE:O	1:C:33:THR:OG1	2.35	0.41
1:C:742:ILE:O	1:C:1000:ARG:NH1	2.43	0.41
1:C:54:LEU:HD21	1:C:88:ASP:HB3	2.01	0.41
1:B:129:LYS:HE3	1:B:169:GLU:HG3	2.02	0.41
1:B:319:ARG:HH11	1:C:740:MET:HE3	1.85	0.41
1:B:821:LEU:O	1:B:825:LYS:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:ILE:HB	4:A:1303:NAG:H5	2.02	0.41
1:C:37:TYR:OH	1:C:54:LEU:O	2.23	0.41
1:C:1084:ASP:OD1	1:C:1084:ASP:N	2.51	0.41
1:B:106:PHE:HB2	1:B:117:LEU:HB3	2.02	0.41
1:A:1142:GLN:HB3	1:A:1143:PRO:HD3	2.02	0.41
1:C:900:MET:HE2	1:C:900:MET:HB3	1.75	0.41
1:B:342:PHE:HE2	1:B:434:ILE:HG21	1.84	0.41
1:C:518:LEU:O	1:C:519:HIS:ND1	2.53	0.41
1:B:108:THR:HG23	1:B:109:THR:HG23	2.03	0.41
1:B:277:LEU:HD12	1:B:285:ILE:HG21	2.02	0.41
1:A:748:GLU:O	1:A:752:LEU:HG	2.20	0.41
1:A:1048:HIS:HA	1:A:1066:THR:HG22	2.02	0.41
1:C:105:ILE:HG22	1:C:118:LEU:HG	2.03	0.41
1:B:127:VAL:HG22	1:B:171:VAL:HG22	2.02	0.41
1:A:96:GLU:HG2	1:A:100:ILE:H	1.84	0.41
1:C:360:ASN:H	1:C:523:THR:HB	1.86	0.41
1:B:578:ASP:HB3	1:B:581:THR:O	2.21	0.40
1:A:404:GLY:HA2	1:A:508:TYR:HD2	1.86	0.40
1:B:360:ASN:H	1:B:523:THR:HB	1.86	0.40
1:C:65:PHE:CE2	1:C:84:LEU:HD11	2.56	0.40
1:A:344:ALA:HB3	1:A:347:PHE:CE1	2.55	0.40
1:A:1116:THR:HG22	1:A:1138:TYR:HB3	2.03	0.40
1:B:886:TRP:HZ3	1:B:905:ARG:HD3	1.86	0.40
1:A:37:TYR:OH	1:A:54:LEU:O	2.37	0.40
1:A:396:TYR:OH	1:A:516:GLU:OE2	2.25	0.40
1:C:886:TRP:HH2	1:C:904:TYR:HB3	1.87	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	1060/1275 (83%)	1025 (97%)	35 (3%)	0	100	100
1	B	1060/1275 (83%)	1025 (97%)	35 (3%)	0	100	100
1	C	1037/1275 (81%)	1010 (97%)	27 (3%)	0	100	100
2	D	16/19 (84%)	15 (94%)	1 (6%)	0	100	100
2	E	16/19 (84%)	16 (100%)	0	0	100	100
2	F	16/19 (84%)	16 (100%)	0	0	100	100
All	All	3205/3882 (83%)	3107 (97%)	98 (3%)	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	920/1102 (84%)	920 (100%)	0	100	100
1	B	922/1102 (84%)	922 (100%)	0	100	100
1	C	907/1102 (82%)	907 (100%)	0	100	100
2	D	15/15 (100%)	15 (100%)	0	100	100
2	E	15/15 (100%)	15 (100%)	0	100	100
2	F	15/15 (100%)	15 (100%)	0	100	100
All	All	2794/3351 (83%)	2794 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	66	HIS
1	B	134	GLN
1	B	173	GLN
1	B	188	ASN
1	B	498	GLN

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Mol	Chain	Res	Type
1	B	992	GLN
1	B	1101	HIS
2	D	7	GLN
1	A	218	GLN
1	A	409	GLN
1	A	536	ASN
1	A	955	ASN
1	C	30	ASN
1	C	165	ASN
1	C	1002	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

3 non-standard protein/DNA/RNA residues 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	CCS	E	17	2	7,8,10	0.79	0	4,8,12	0.84	0
2	CCS	D	17	2	7,8,10	0.78	0	4,8,12	1.04	0
2	CCS	F	17	2	7,8,10	0.79	0	4,8,12	0.60	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	CCS	E	17	2	-	0/4/7/10	-
2	CCS	D	17	2	-	0/4/7/10	-
2	CCS	F	17	2	-	0/4/7/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

26 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	G	1	3,1	14,14,15	0.26	0	17,19,21	0.48	0
3	NAG	G	2	3	14,14,15	0.24	0	17,19,21	0.43	0
3	NAG	H	1	3,1	14,14,15	0.21	0	17,19,21	0.49	0
3	NAG	H	2	3	14,14,15	0.21	0	17,19,21	0.40	0
3	NAG	I	1	3,1	14,14,15	0.22	0	17,19,21	0.48	0
3	NAG	I	2	3	14,14,15	0.22	0	17,19,21	0.44	0
3	NAG	J	1	3,1	14,14,15	0.22	0	17,19,21	0.46	0
3	NAG	J	2	3	14,14,15	0.22	0	17,19,21	0.40	0
3	NAG	K	1	3,1	14,14,15	0.21	0	17,19,21	0.40	0
3	NAG	K	2	3	14,14,15	0.26	0	17,19,21	0.58	0
3	NAG	L	1	3,1	14,14,15	0.29	0	17,19,21	0.59	0
3	NAG	L	2	3	14,14,15	0.25	0	17,19,21	0.44	0
3	NAG	M	1	3,1	14,14,15	0.35	0	17,19,21	0.51	0
3	NAG	M	2	3	14,14,15	0.23	0	17,19,21	0.47	0
3	NAG	N	1	3,1	14,14,15	0.19	0	17,19,21	0.50	0
3	NAG	N	2	3	14,14,15	0.23	0	17,19,21	0.44	0
3	NAG	O	1	3,1	14,14,15	0.25	0	17,19,21	0.46	0
3	NAG	O	2	3	14,14,15	0.25	0	17,19,21	0.40	0
3	NAG	P	1	3,1	14,14,15	0.21	0	17,19,21	0.46	0
3	NAG	P	2	3	14,14,15	0.22	0	17,19,21	0.44	0
3	NAG	Q	1	3,1	14,14,15	0.21	0	17,19,21	0.49	0
3	NAG	Q	2	3	14,14,15	0.22	0	17,19,21	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	R	1	3,1	14,14,15	0.22	0	17,19,21	0.53	0
3	NAG	R	2	3	14,14,15	0.23	0	17,19,21	0.41	0
3	NAG	S	1	3,1	14,14,15	0.21	0	17,19,21	0.43	0
3	NAG	S	2	3	14,14,15	0.21	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	G	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	G	2	3	-	0/6/23/26	0/1/1/1
3	NAG	H	1	3,1	-	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	3,1	-	2/6/23/26	0/1/1/1
3	NAG	I	2	3	-	3/6/23/26	0/1/1/1
3	NAG	J	1	3,1	-	3/6/23/26	0/1/1/1
3	NAG	J	2	3	-	2/6/23/26	0/1/1/1
3	NAG	K	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	K	2	3	-	4/6/23/26	0/1/1/1
3	NAG	L	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	L	2	3	-	2/6/23/26	0/1/1/1
3	NAG	M	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	M	2	3	-	0/6/23/26	0/1/1/1
3	NAG	N	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	N	2	3	-	2/6/23/26	0/1/1/1
3	NAG	O	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	O	2	3	-	2/6/23/26	0/1/1/1
3	NAG	P	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	P	2	3	-	2/6/23/26	0/1/1/1
3	NAG	Q	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	2/6/23/26	0/1/1/1
3	NAG	R	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	R	2	3	-	3/6/23/26	0/1/1/1
3	NAG	S	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	S	2	3	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	Q	2	NAG	C4-C5-C6-O6
3	Q	2	NAG	O5-C5-C6-O6
3	K	2	NAG	O5-C5-C6-O6
3	I	1	NAG	O5-C5-C6-O6
3	N	1	NAG	O5-C5-C6-O6
3	N	2	NAG	C4-C5-C6-O6
3	J	2	NAG	C4-C5-C6-O6
3	N	1	NAG	C4-C5-C6-O6
3	O	2	NAG	O5-C5-C6-O6
3	H	1	NAG	O5-C5-C6-O6
3	K	2	NAG	C4-C5-C6-O6
3	J	2	NAG	O5-C5-C6-O6
3	N	2	NAG	O5-C5-C6-O6
3	I	1	NAG	C4-C5-C6-O6
3	O	2	NAG	C4-C5-C6-O6
3	S	2	NAG	O5-C5-C6-O6
3	S	1	NAG	O5-C5-C6-O6
3	S	2	NAG	C4-C5-C6-O6
3	L	2	NAG	O5-C5-C6-O6
3	L	2	NAG	C4-C5-C6-O6
3	I	2	NAG	O5-C5-C6-O6
3	I	2	NAG	C4-C5-C6-O6
3	R	2	NAG	O5-C5-C6-O6
3	R	2	NAG	C4-C5-C6-O6
3	O	1	NAG	C4-C5-C6-O6
3	H	1	NAG	C4-C5-C6-O6
3	P	2	NAG	C4-C5-C6-O6
3	S	1	NAG	C4-C5-C6-O6
3	J	1	NAG	C4-C5-C6-O6
3	L	1	NAG	C4-C5-C6-O6
3	M	1	NAG	C4-C5-C6-O6
3	M	1	NAG	O5-C5-C6-O6
3	O	1	NAG	O5-C5-C6-O6
3	P	2	NAG	O5-C5-C6-O6
3	J	1	NAG	O5-C5-C6-O6
3	K	2	NAG	C3-C2-N2-C7
3	L	1	NAG	O5-C5-C6-O6

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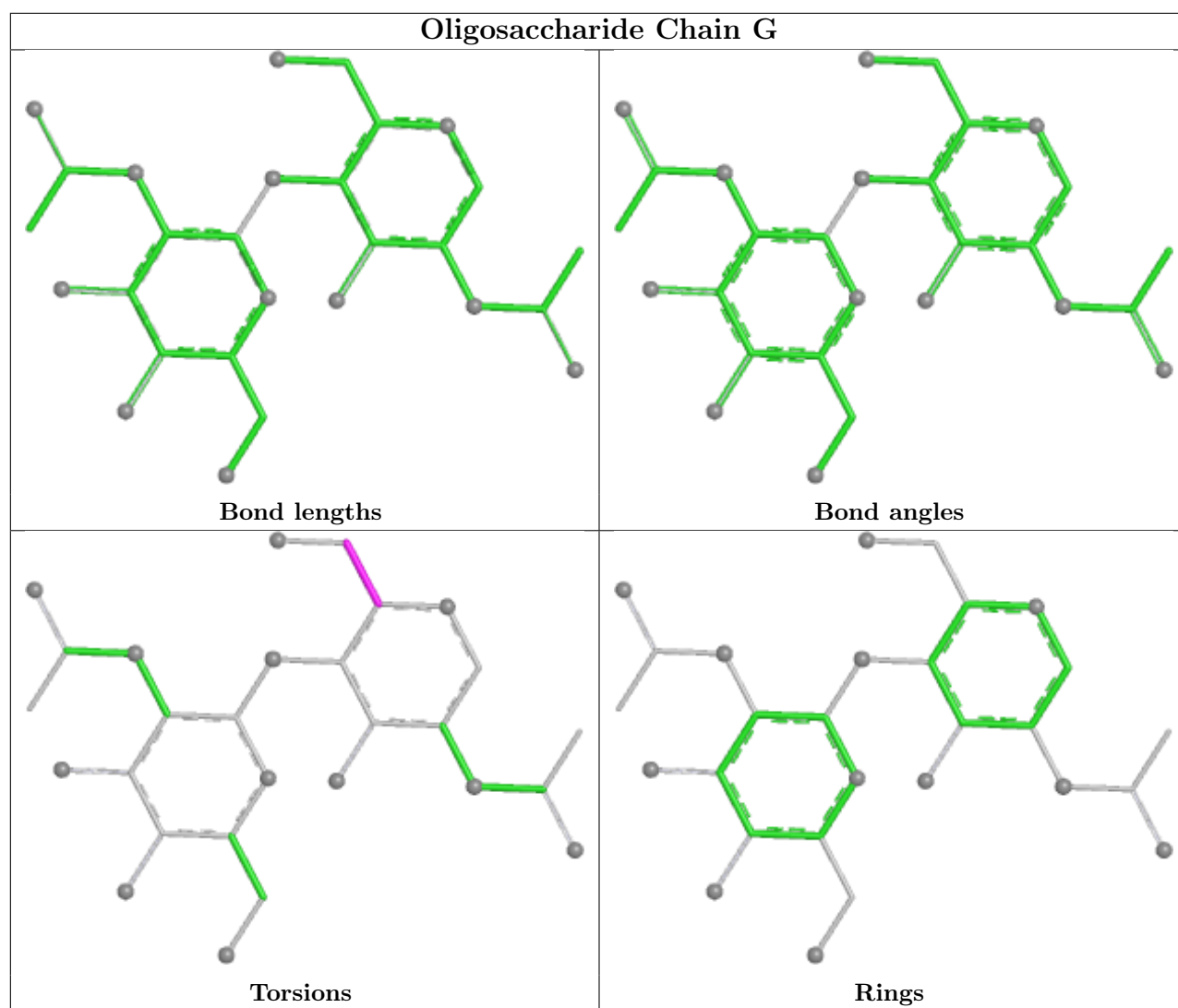
Mol	Chain	Res	Type	Atoms
3	G	1	NAG	O5-C5-C6-O6
3	I	2	NAG	C1-C2-N2-C7
3	J	1	NAG	C1-C2-N2-C7
3	K	2	NAG	C1-C2-N2-C7
3	R	2	NAG	C1-C2-N2-C7

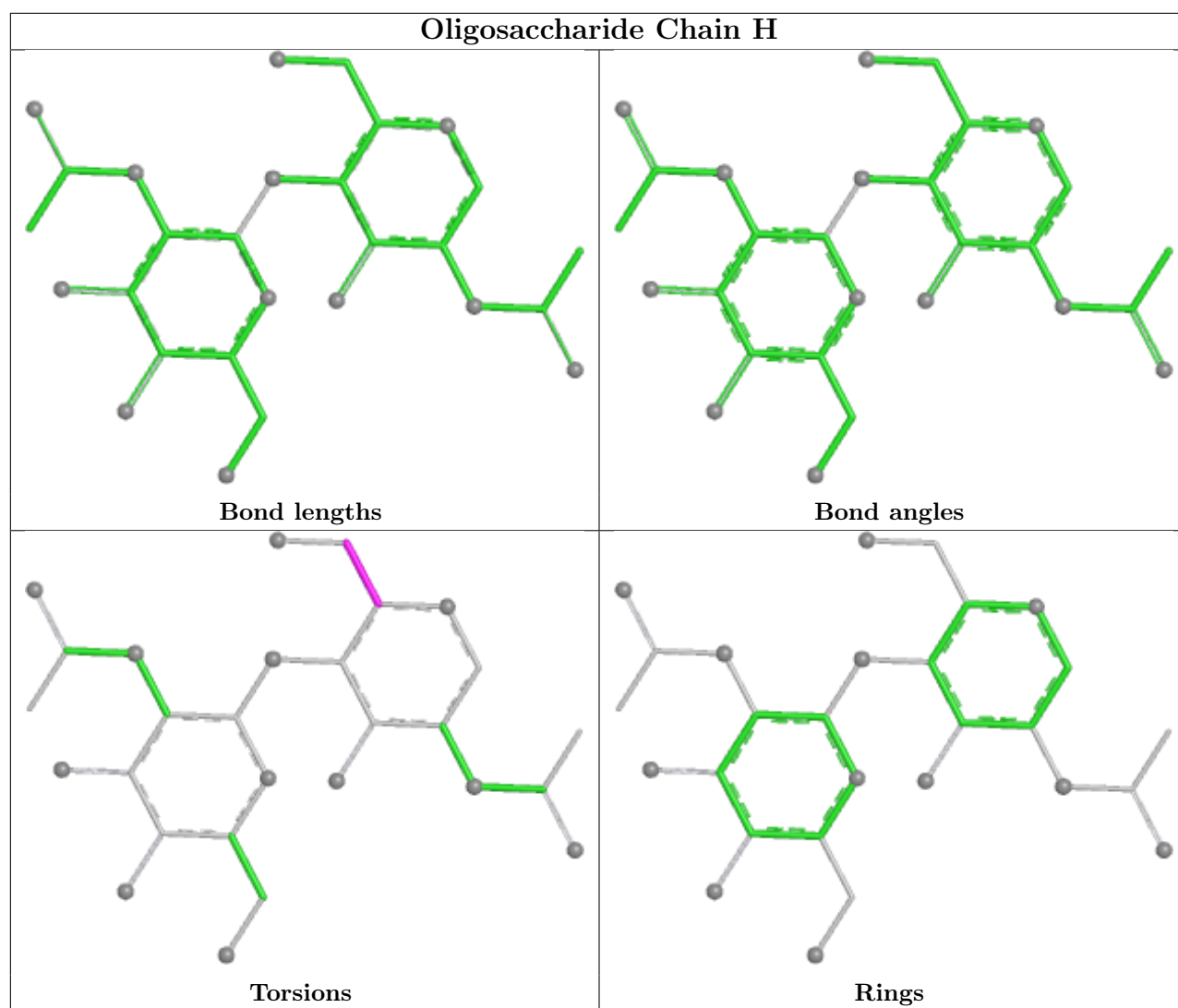
There are no ring outliers.

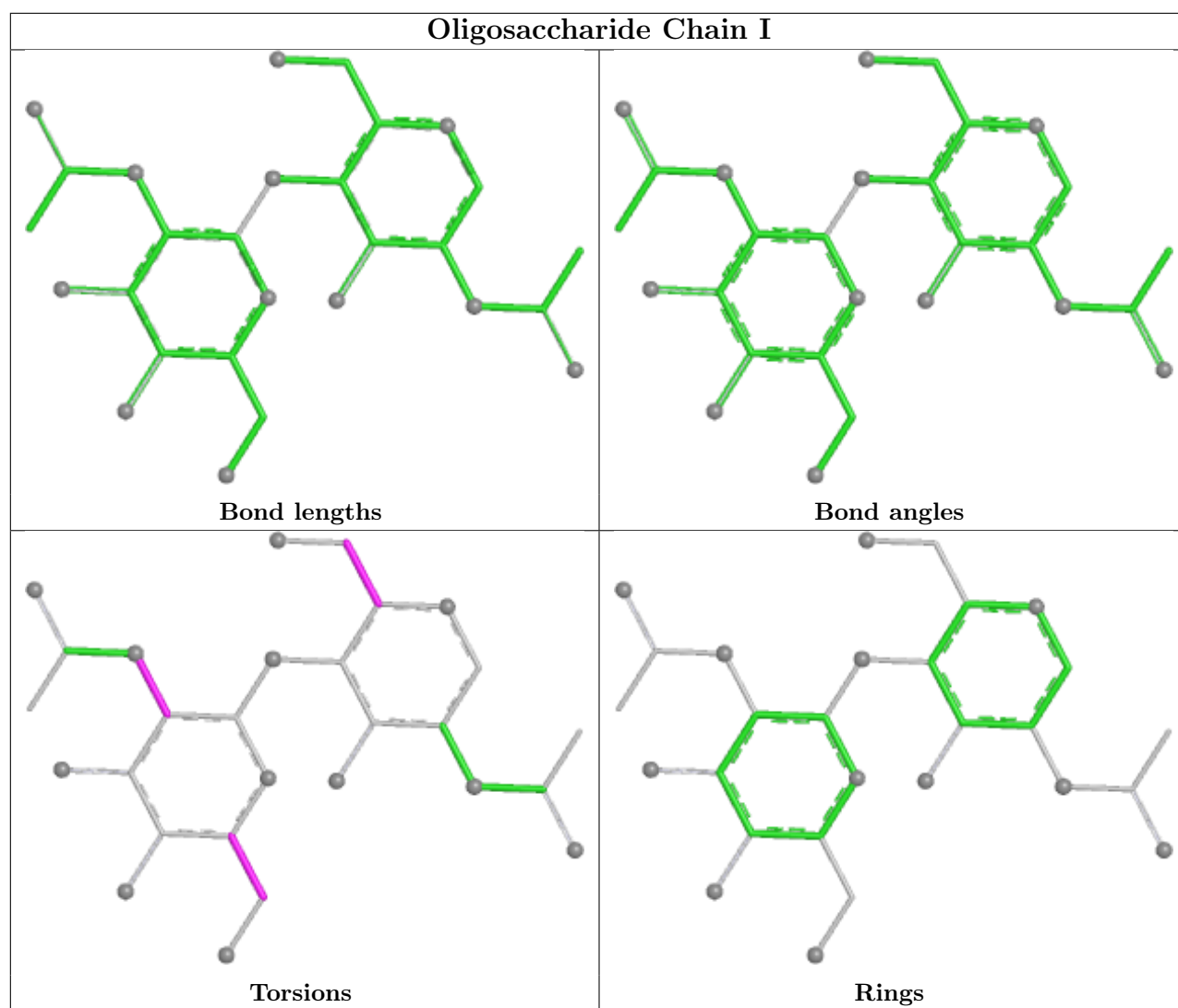
3 monomers are involved in 3 short contacts:

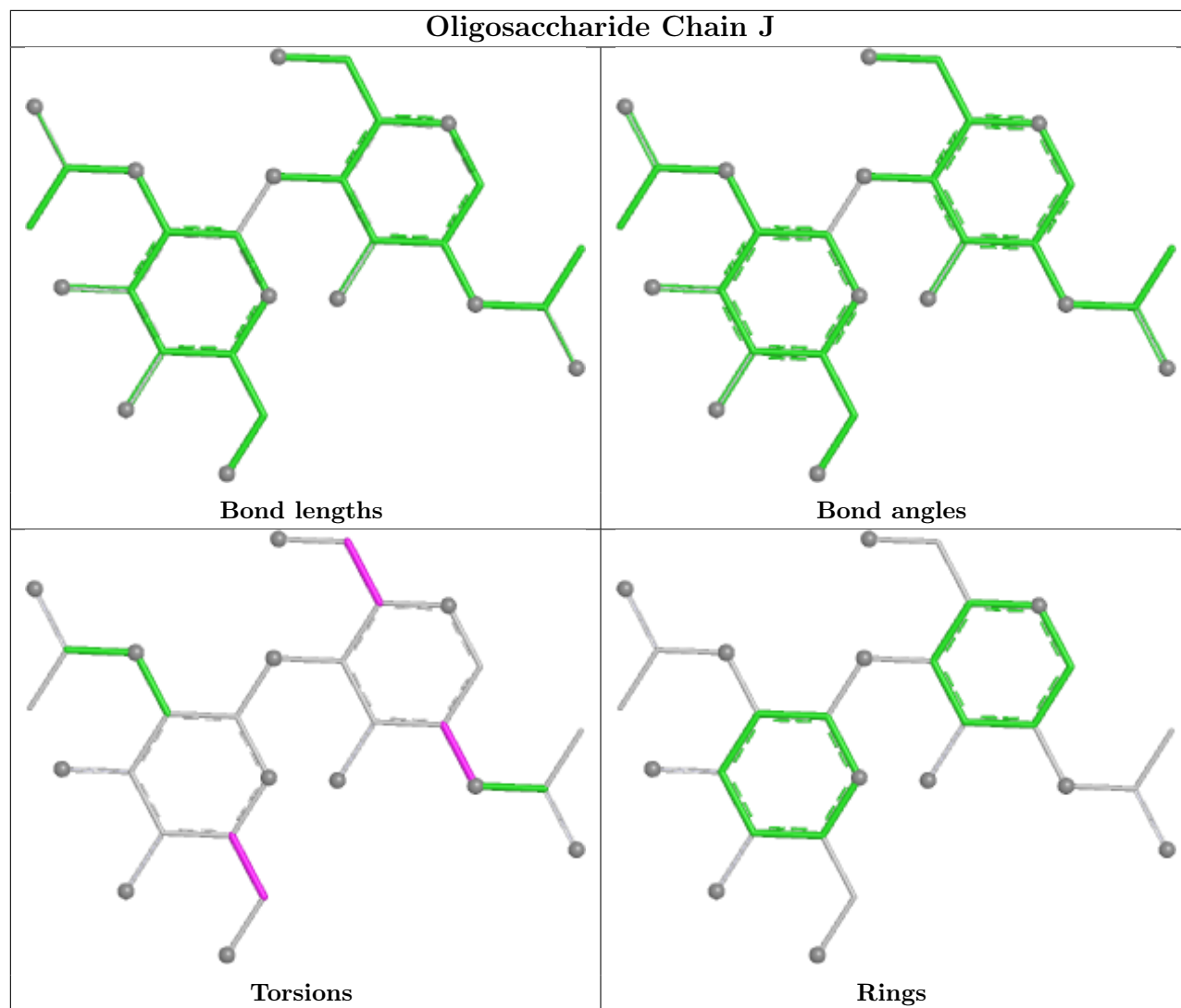
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L	1	NAG	1	0
3	P	1	NAG	1	0
3	M	1	NAG	1	0

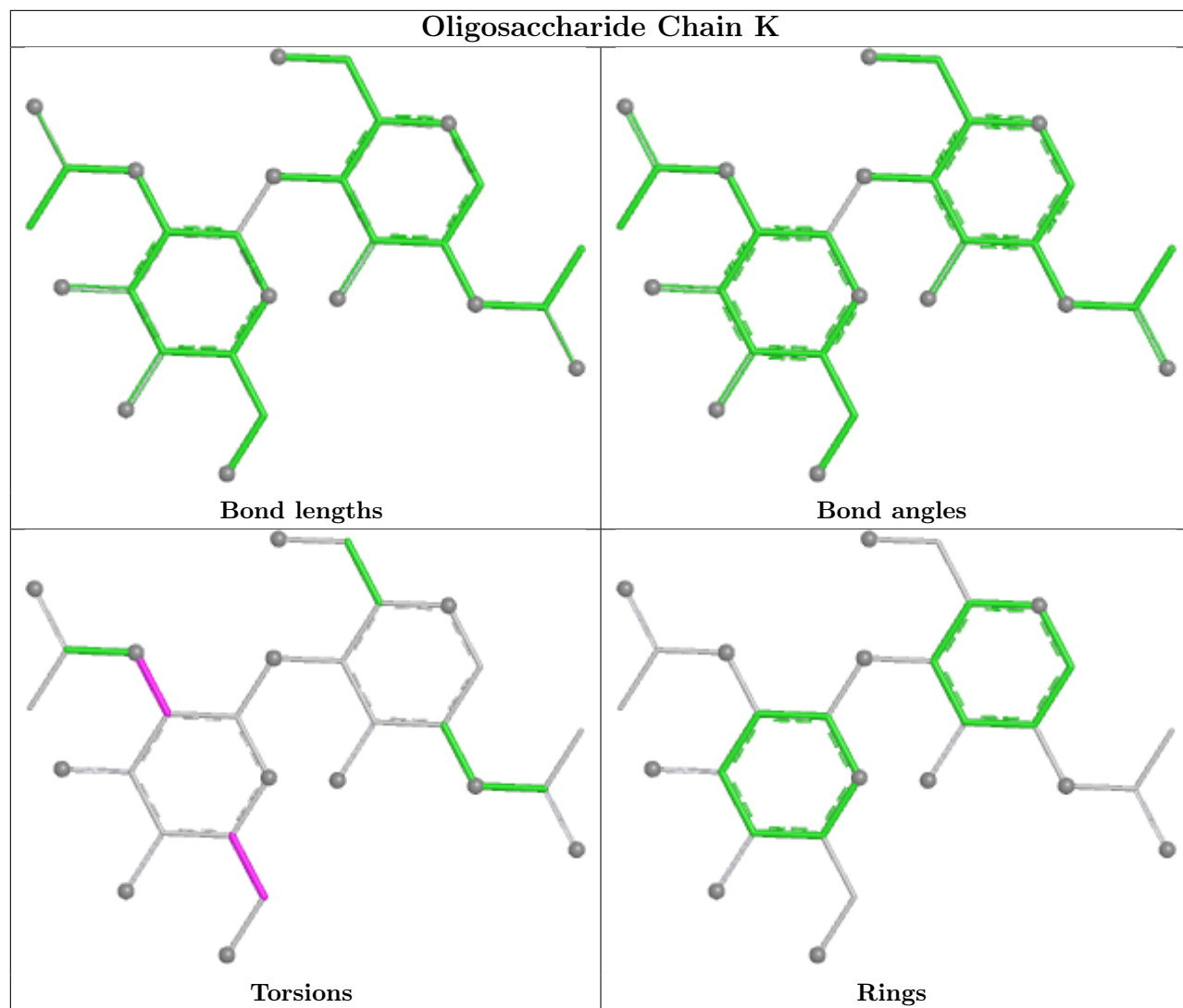
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

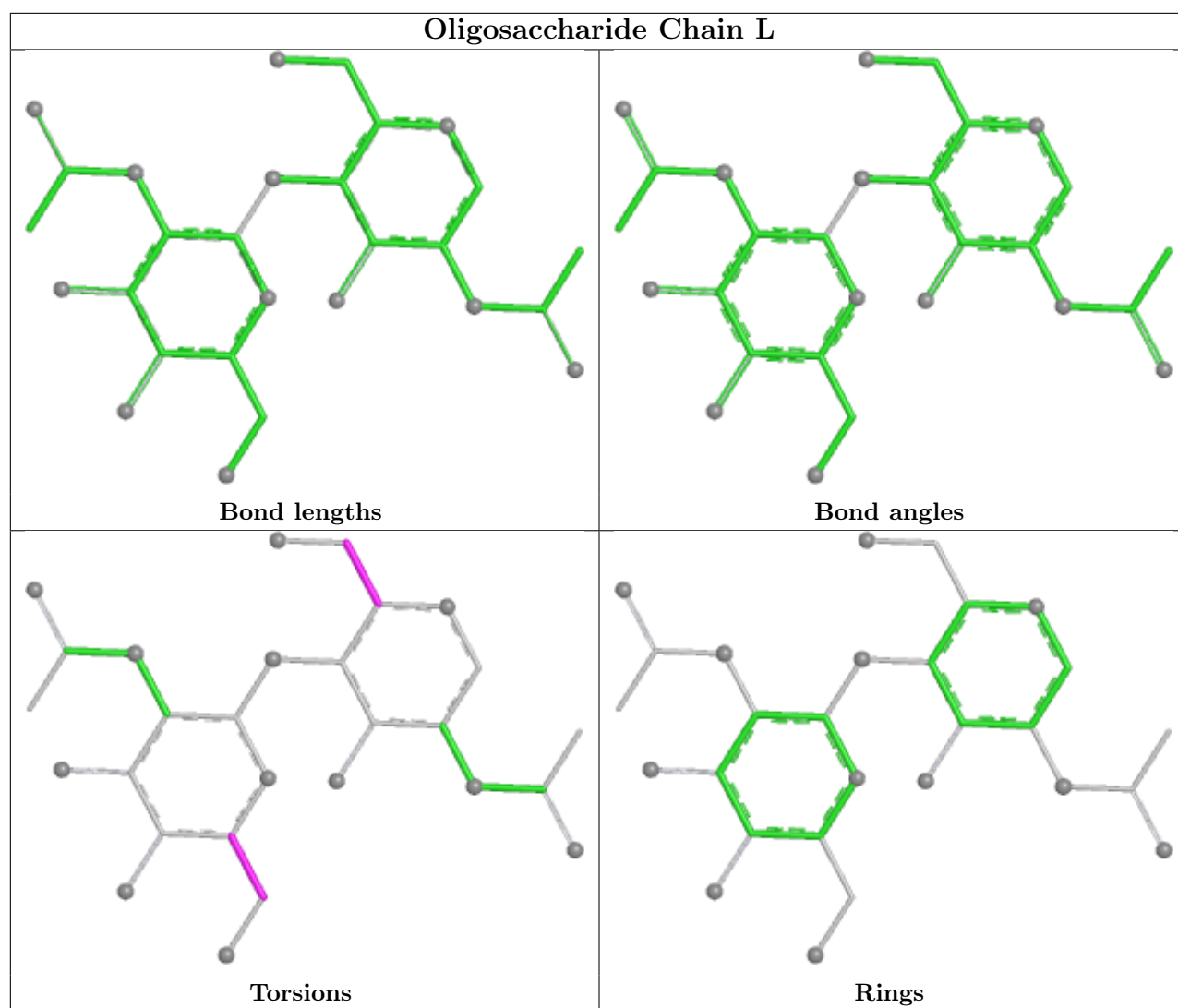


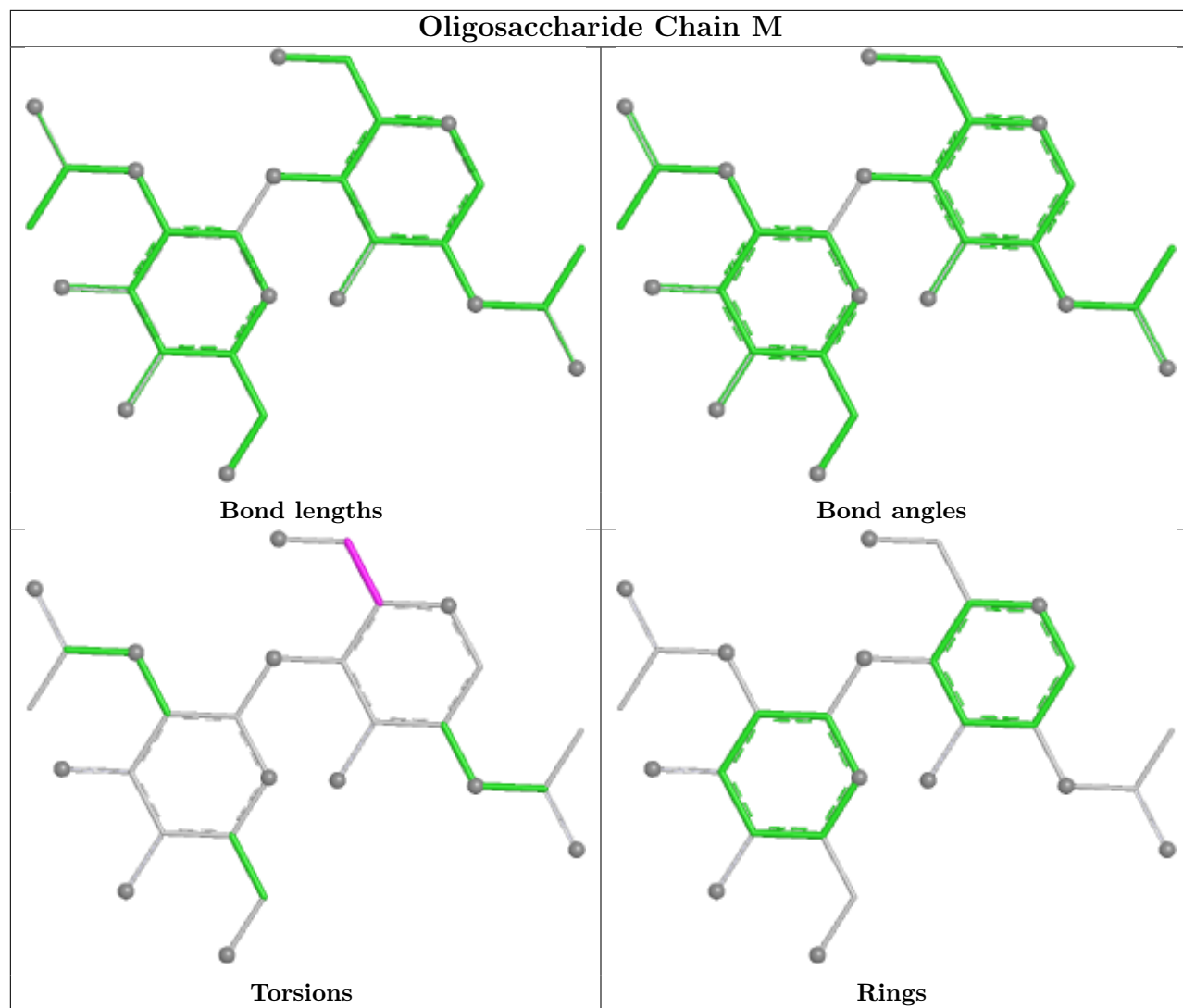


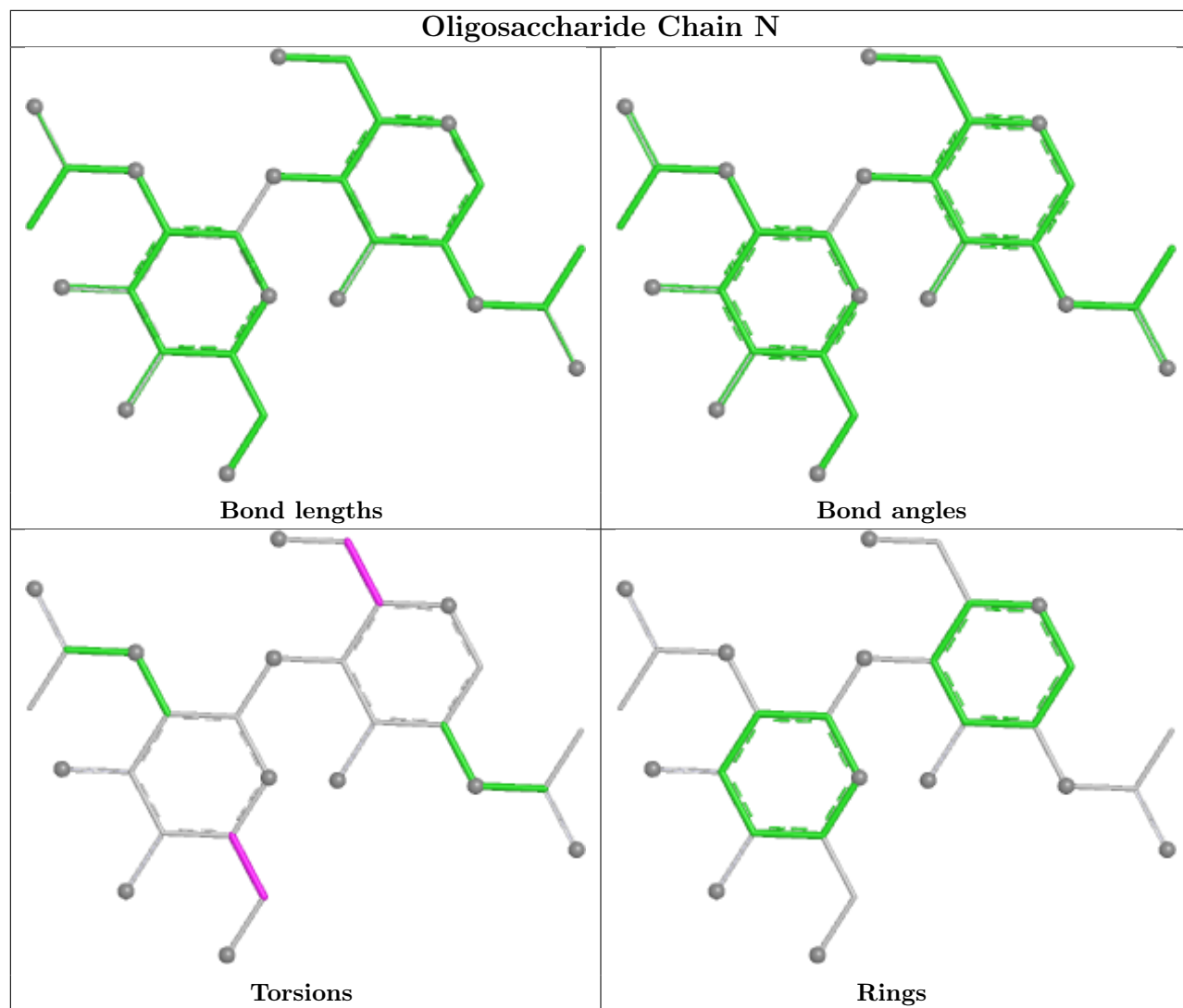


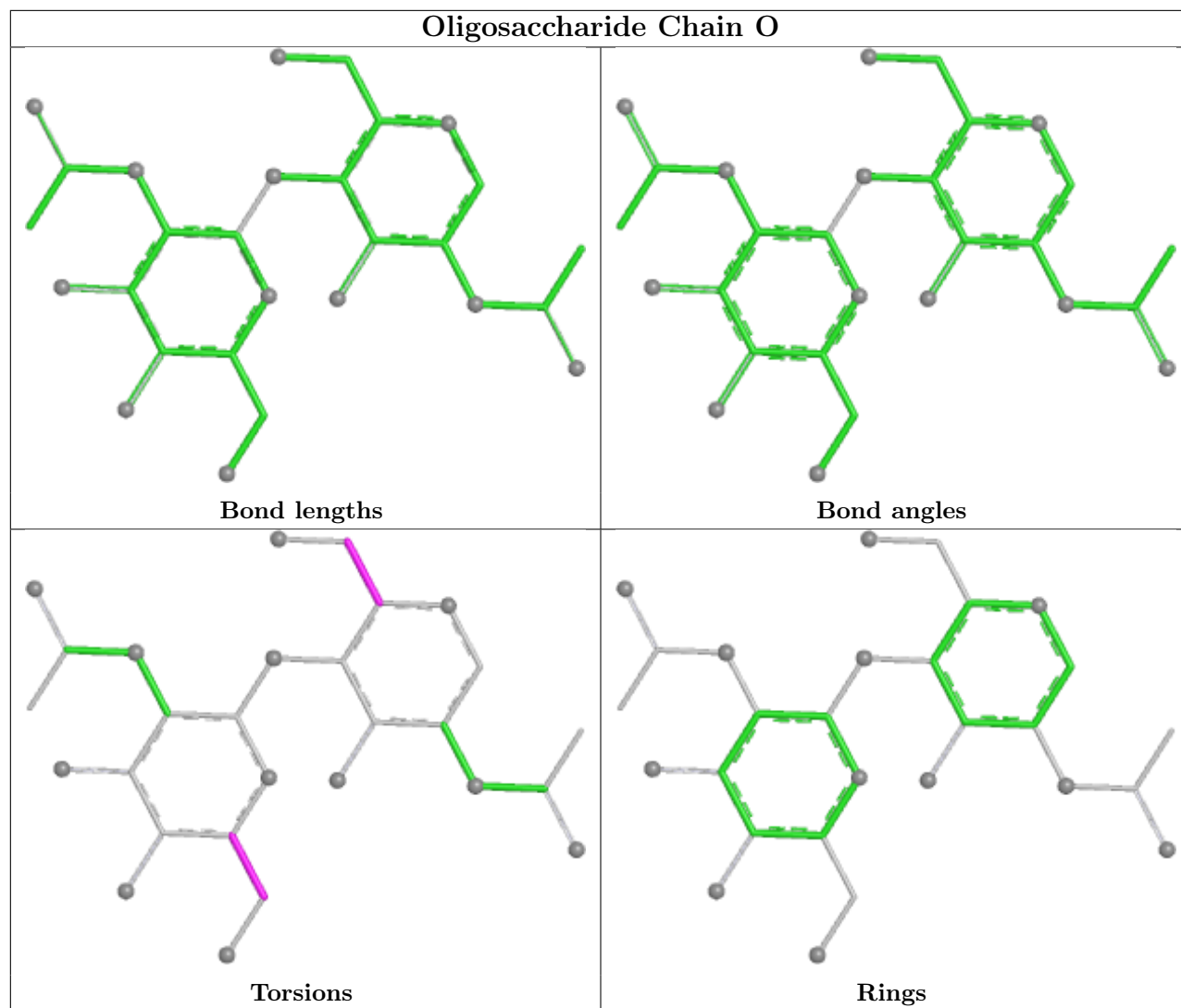


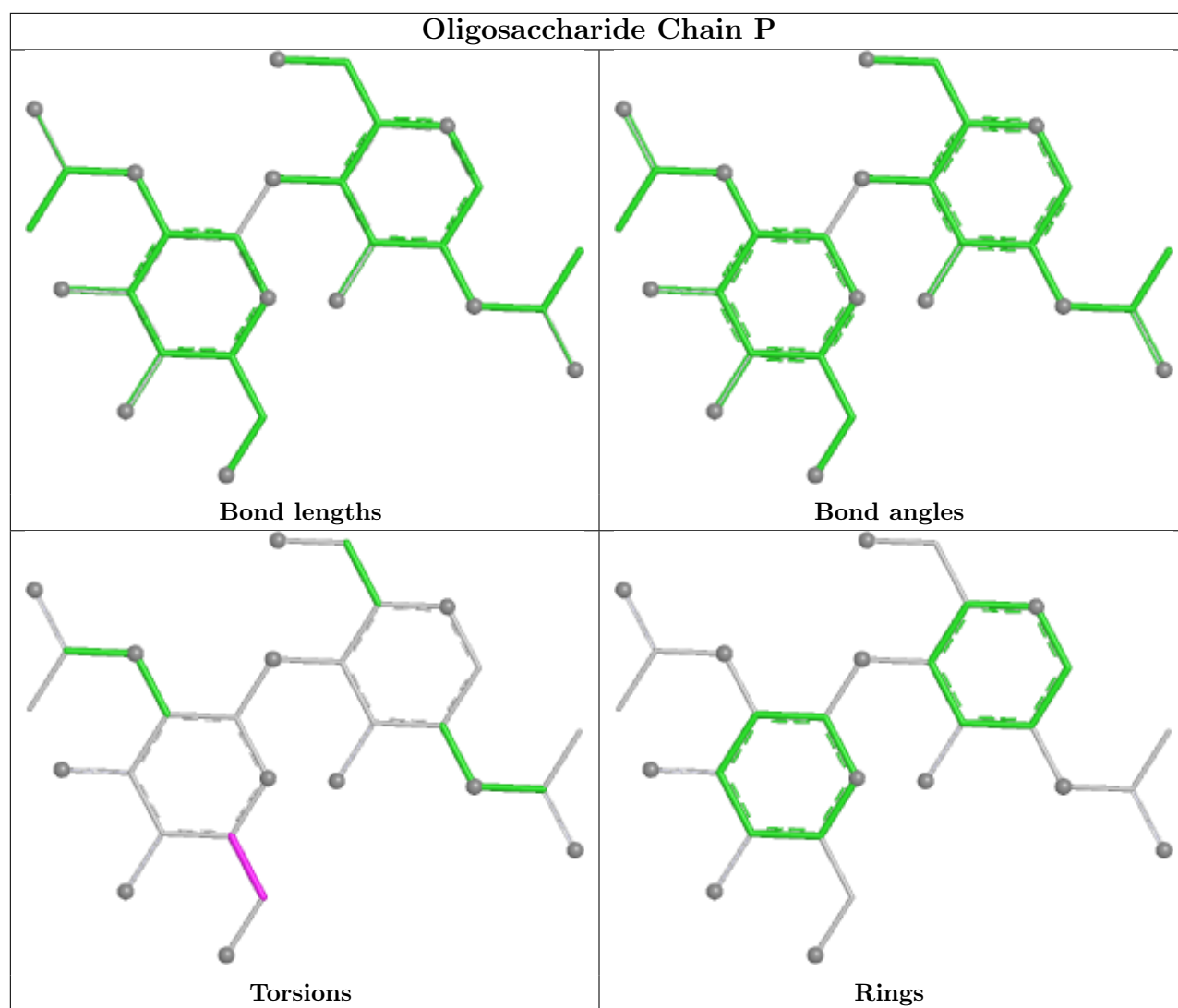


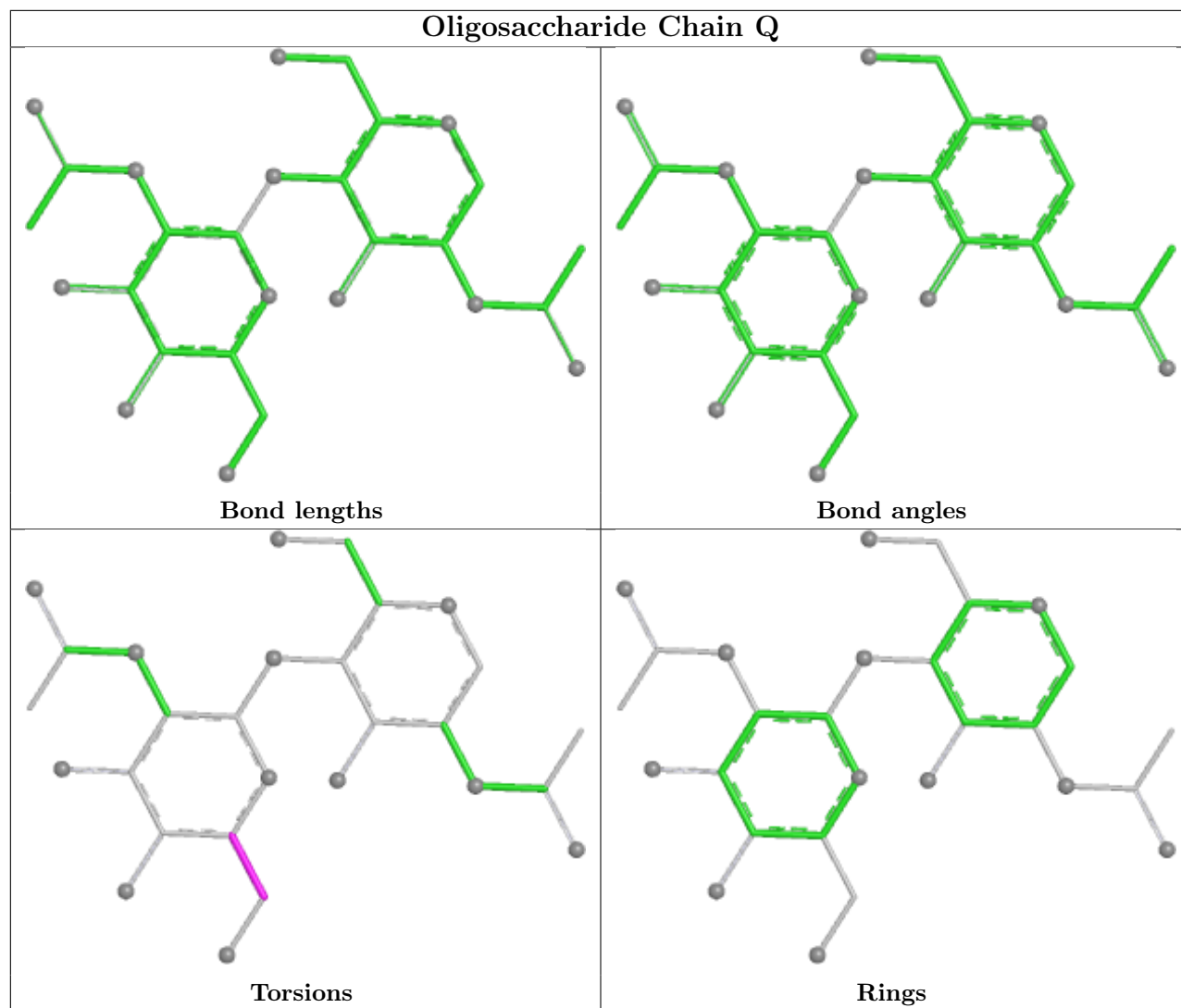


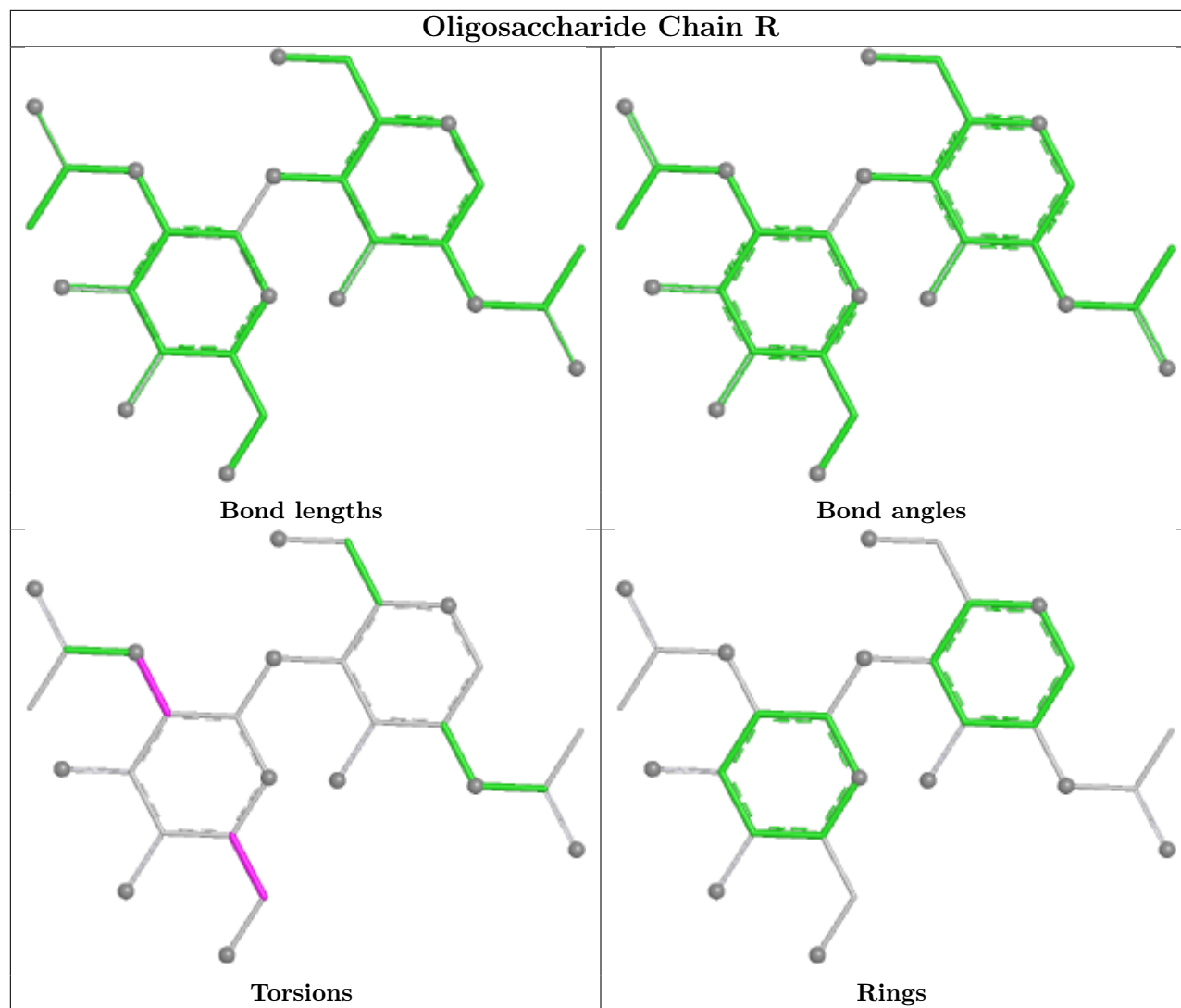


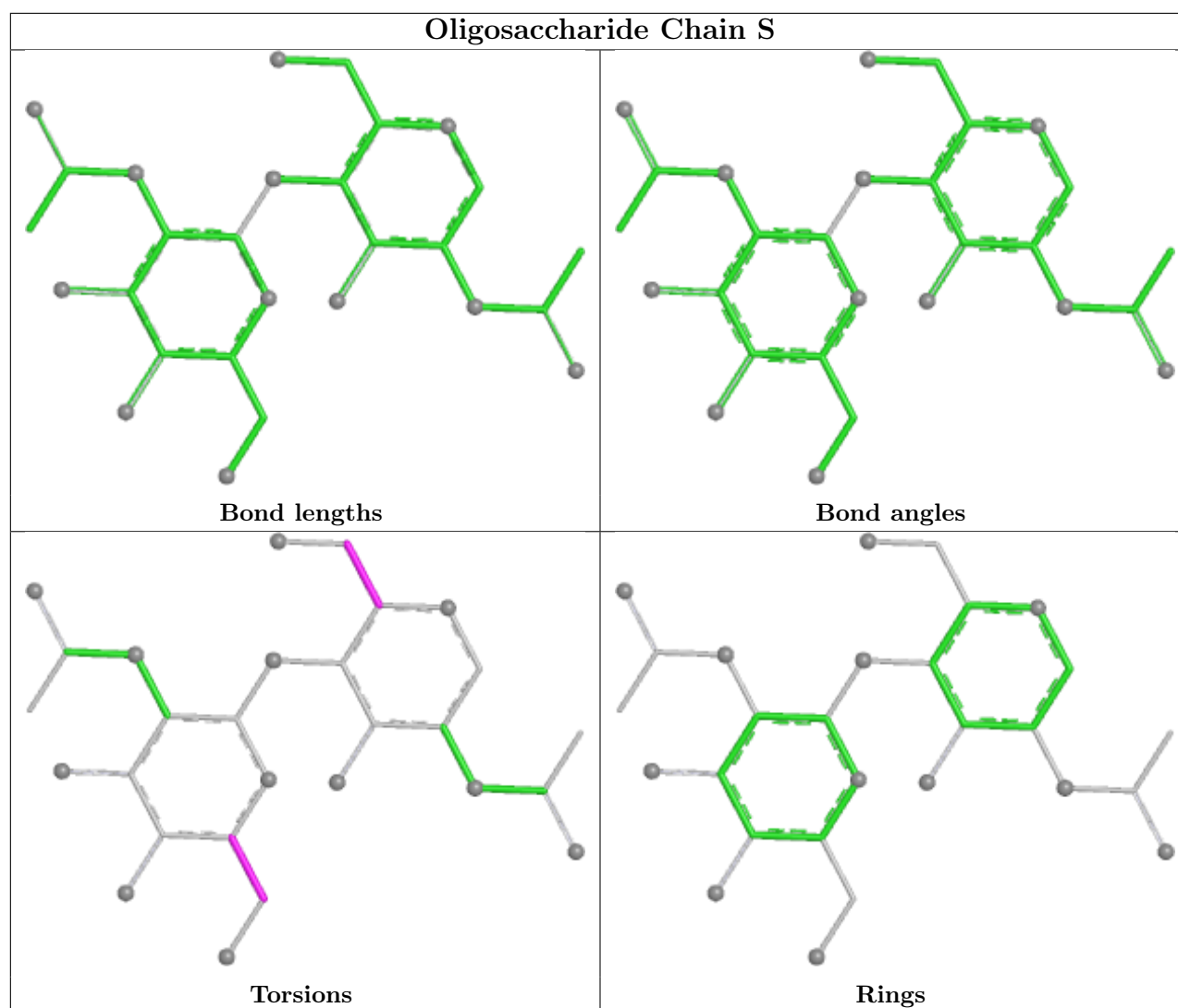












5.6 Ligand geometry [i](#)

23 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	$\# Z > 2$
4	NAG	B	1305	1	14,14,15	0.19	0	17,19,21	0.44	0
4	NAG	B	1303	1	14,14,15	0.25	0	17,19,21	0.47	0
4	NAG	C	1305	1	14,14,15	0.19	0	17,19,21	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	A	1302	1	14,14,15	0.49	0	17,19,21	1.34	2 (11%)
4	NAG	C	1306	1	14,14,15	0.26	0	17,19,21	0.35	0
4	NAG	B	1304	1	14,14,15	0.21	0	17,19,21	0.44	0
4	NAG	A	1306	-	14,14,15	0.23	0	17,19,21	0.41	0
4	NAG	A	1304	1	14,14,15	0.34	0	17,19,21	0.43	0
4	NAG	C	1301	1	14,14,15	0.22	0	17,19,21	0.50	0
4	NAG	A	1301	1	14,14,15	0.22	0	17,19,21	0.45	0
4	NAG	B	1302	1	14,14,15	0.26	0	17,19,21	0.41	0
4	NAG	C	1309	1	14,14,15	0.24	0	17,19,21	0.45	0
4	NAG	C	1308	1	14,14,15	0.46	0	17,19,21	1.34	2 (11%)
4	NAG	B	1306	1	14,14,15	0.23	0	17,19,21	0.36	0
4	NAG	B	1301	1	14,14,15	0.23	0	17,19,21	0.42	0
4	NAG	A	1307	1	14,14,15	0.22	0	17,19,21	0.44	0
4	NAG	A	1308	1	14,14,15	0.21	0	17,19,21	0.43	0
4	NAG	C	1304	1	14,14,15	0.22	0	17,19,21	0.42	0
4	NAG	C	1302	1	14,14,15	0.23	0	17,19,21	0.43	0
4	NAG	A	1305	1	14,14,15	0.19	0	17,19,21	0.41	0
4	NAG	C	1307	1	14,14,15	0.31	0	17,19,21	0.39	0
4	NAG	C	1303	1	14,14,15	0.20	0	17,19,21	0.47	0
4	NAG	A	1303	-	14,14,15	0.62	0	17,19,21	1.25	3 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	1305	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1303	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1305	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1302	1	-	6/6/23/26	0/1/1/1
4	NAG	C	1306	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1304	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1306	-	-	2/6/23/26	0/1/1/1
4	NAG	A	1304	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1301	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1301	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1302	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1309	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1308	1	-	6/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	1306	1	-	4/6/23/26	0/1/1/1
4	NAG	B	1301	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1307	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1308	1	-	4/6/23/26	0/1/1/1
4	NAG	C	1304	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1302	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1305	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1307	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1303	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1303	-	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1308	NAG	C2-N2-C7	4.58	129.03	122.90
4	A	1302	NAG	C2-N2-C7	4.57	129.03	122.90
4	A	1303	NAG	C2-N2-C7	2.95	126.85	122.90
4	A	1303	NAG	C1-O5-C5	2.66	115.75	112.19
4	A	1303	NAG	C1-C2-N2	2.47	114.32	110.43
4	C	1308	NAG	C1-C2-N2	2.19	113.88	110.43
4	A	1302	NAG	C1-C2-N2	2.11	113.75	110.43

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1302	NAG	C4-C5-C6-O6
4	A	1308	NAG	C4-C5-C6-O6
4	C	1306	NAG	O5-C5-C6-O6
4	C	1307	NAG	C4-C5-C6-O6
4	B	1301	NAG	O5-C5-C6-O6
4	A	1301	NAG	O5-C5-C6-O6
4	A	1305	NAG	O5-C5-C6-O6
4	C	1309	NAG	O5-C5-C6-O6
4	B	1306	NAG	C4-C5-C6-O6
4	B	1301	NAG	C4-C5-C6-O6
4	B	1305	NAG	O5-C5-C6-O6
4	A	1305	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	C	1306	NAG	C4-C5-C6-O6
4	A	1307	NAG	O5-C5-C6-O6
4	B	1306	NAG	O5-C5-C6-O6
4	A	1302	NAG	O5-C5-C6-O6
4	A	1308	NAG	O5-C5-C6-O6
4	A	1306	NAG	C4-C5-C6-O6
4	B	1304	NAG	O5-C5-C6-O6
4	A	1307	NAG	C4-C5-C6-O6
4	C	1307	NAG	O5-C5-C6-O6
4	C	1309	NAG	C4-C5-C6-O6
4	B	1305	NAG	C4-C5-C6-O6
4	A	1306	NAG	O5-C5-C6-O6
4	A	1301	NAG	C4-C5-C6-O6
4	B	1304	NAG	C4-C5-C6-O6
4	B	1303	NAG	C8-C7-N2-C2
4	B	1303	NAG	O7-C7-N2-C2
4	B	1306	NAG	C8-C7-N2-C2
4	B	1306	NAG	O7-C7-N2-C2
4	A	1302	NAG	C8-C7-N2-C2
4	A	1302	NAG	O7-C7-N2-C2
4	A	1308	NAG	C8-C7-N2-C2
4	A	1308	NAG	O7-C7-N2-C2
4	C	1308	NAG	C8-C7-N2-C2
4	C	1308	NAG	O7-C7-N2-C2
4	C	1308	NAG	O5-C5-C6-O6
4	A	1303	NAG	O5-C5-C6-O6
4	C	1301	NAG	C4-C5-C6-O6
4	C	1301	NAG	O5-C5-C6-O6
4	C	1303	NAG	C4-C5-C6-O6
4	C	1302	NAG	O5-C5-C6-O6
4	C	1303	NAG	O5-C5-C6-O6
4	C	1305	NAG	O5-C5-C6-O6
4	A	1303	NAG	C3-C2-N2-C7
4	C	1304	NAG	O5-C5-C6-O6
4	C	1308	NAG	C4-C5-C6-O6
4	A	1302	NAG	C1-C2-N2-C7
4	C	1308	NAG	C1-C2-N2-C7
4	A	1302	NAG	C3-C2-N2-C7
4	C	1308	NAG	C3-C2-N2-C7
4	A	1303	NAG	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1302	NAG	1	0
4	C	1308	NAG	1	0
4	A	1303	NAG	4	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.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-16144. 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.