



## Full wwPDB EM Validation Report ⓘ

Nov 13, 2024 – 10:42 AM JST

PDB ID : 8WLY  
EMDB ID : EMD-37635  
Title : Cryo-EM structure of bat WIV1 spike glycoprotein  
Authors : Wang, X.; Qiao, S.  
Deposited on : 2023-10-01  
Resolution : 3.96 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>.

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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 : 4.02b-467  
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) : 2.39

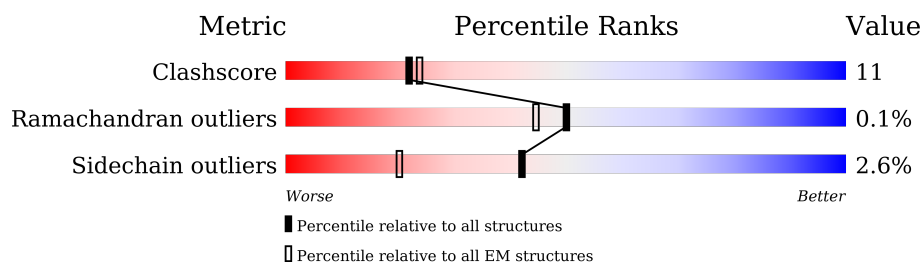
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.96 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	1271	49% 19% 32%
1	B	1271	61% 22% 16%
1	C	1271	51% 17% 31%
2	D	2	100%
2	E	2	50% 50%
2	F	2	50% 50%
2	G	2	100%
2	H	2	50% 50%
2	I	2	50% 50%

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Mol	Chain	Length	Quality of chain
2	J	2	 50%50%
2	M	2	 100%
2	N	2	 50%50%
2	O	2	 50%50%
2	P	2	 100%
2	R	2	 50%50%
2	S	2	 100%
3	K	3	 100%
3	L	3	 100%
3	Q	3	 33%67%

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 22598 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	A	870	Total	C	N	O	S	0	0
			6757	4303	1128	1293	33		
1	B	1067	Total	C	N	O	S	0	0
			8325	5312	1386	1586	41		
1	C	871	Total	C	N	O	S	0	0
			6769	4312	1129	1295	33		

There are 168 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	969	PRO	LYS	conflict	UNP U5WI05
A	970	PRO	VAL	conflict	UNP U5WI05
A	1192	GLY	-	linker	UNP U5WI05
A	1193	SER	-	linker	UNP U5WI05
A	1220	LEU	-	expression tag	UNP A0A346FJN8
A	1221	GLY	-	expression tag	UNP A0A346FJN8
A	1222	ARG	-	expression tag	UNP A0A346FJN8
A	1223	SER	-	expression tag	UNP A0A346FJN8
A	1224	LEU	-	expression tag	UNP A0A346FJN8
A	1225	GLU	-	expression tag	UNP A0A346FJN8
A	1226	VAL	-	expression tag	UNP A0A346FJN8
A	1227	LEU	-	expression tag	UNP A0A346FJN8
A	1228	PHE	-	expression tag	UNP A0A346FJN8
A	1229	GLN	-	expression tag	UNP A0A346FJN8
A	1230	GLY	-	expression tag	UNP A0A346FJN8
A	1231	PRO	-	expression tag	UNP A0A346FJN8
A	1232	GLY	-	expression tag	UNP A0A346FJN8
A	1233	HIS	-	expression tag	UNP A0A346FJN8
A	1234	HIS	-	expression tag	UNP A0A346FJN8
A	1235	HIS	-	expression tag	UNP A0A346FJN8
A	1236	HIS	-	expression tag	UNP A0A346FJN8
A	1237	HIS	-	expression tag	UNP A0A346FJN8
A	1238	HIS	-	expression tag	UNP A0A346FJN8
A	1239	HIS	-	expression tag	UNP A0A346FJN8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1240	HIS	-	expression tag	UNP A0A346FJN8
A	1241	SER	-	expression tag	UNP A0A346FJN8
A	1242	ALA	-	expression tag	UNP A0A346FJN8
A	1243	TRP	-	expression tag	UNP A0A346FJN8
A	1244	SER	-	expression tag	UNP A0A346FJN8
A	1245	HIS	-	expression tag	UNP A0A346FJN8
A	1246	PRO	-	expression tag	UNP A0A346FJN8
A	1247	GLN	-	expression tag	UNP A0A346FJN8
A	1248	PHE	-	expression tag	UNP A0A346FJN8
A	1249	GLU	-	expression tag	UNP A0A346FJN8
A	1250	LYS	-	expression tag	UNP A0A346FJN8
A	1251	GLY	-	expression tag	UNP A0A346FJN8
A	1252	GLY	-	expression tag	UNP A0A346FJN8
A	1253	GLY	-	expression tag	UNP A0A346FJN8
A	1254	SER	-	expression tag	UNP A0A346FJN8
A	1255	GLY	-	expression tag	UNP A0A346FJN8
A	1256	GLY	-	expression tag	UNP A0A346FJN8
A	1257	GLY	-	expression tag	UNP A0A346FJN8
A	1258	GLY	-	expression tag	UNP A0A346FJN8
A	1259	SER	-	expression tag	UNP A0A346FJN8
A	1260	GLY	-	expression tag	UNP A0A346FJN8
A	1261	GLY	-	expression tag	UNP A0A346FJN8
A	1262	SER	-	expression tag	UNP A0A346FJN8
A	1263	ALA	-	expression tag	UNP A0A346FJN8
A	1264	TRP	-	expression tag	UNP A0A346FJN8
A	1265	SER	-	expression tag	UNP A0A346FJN8
A	1266	HIS	-	expression tag	UNP A0A346FJN8
A	1267	PRO	-	expression tag	UNP A0A346FJN8
A	1268	GLN	-	expression tag	UNP A0A346FJN8
A	1269	PHE	-	expression tag	UNP A0A346FJN8
A	1270	GLU	-	expression tag	UNP A0A346FJN8
A	1271	LYS	-	expression tag	UNP A0A346FJN8
B	969	PRO	LYS	conflict	UNP U5WI05
B	970	PRO	VAL	conflict	UNP U5WI05
B	1192	GLY	-	linker	UNP U5WI05
B	1193	SER	-	linker	UNP U5WI05
B	1220	LEU	-	expression tag	UNP A0A346FJN8
B	1221	GLY	-	expression tag	UNP A0A346FJN8
B	1222	ARG	-	expression tag	UNP A0A346FJN8
B	1223	SER	-	expression tag	UNP A0A346FJN8
B	1224	LEU	-	expression tag	UNP A0A346FJN8
B	1225	GLU	-	expression tag	UNP A0A346FJN8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1226	VAL	-	expression tag	UNP A0A346FJN8
B	1227	LEU	-	expression tag	UNP A0A346FJN8
B	1228	PHE	-	expression tag	UNP A0A346FJN8
B	1229	GLN	-	expression tag	UNP A0A346FJN8
B	1230	GLY	-	expression tag	UNP A0A346FJN8
B	1231	PRO	-	expression tag	UNP A0A346FJN8
B	1232	GLY	-	expression tag	UNP A0A346FJN8
B	1233	HIS	-	expression tag	UNP A0A346FJN8
B	1234	HIS	-	expression tag	UNP A0A346FJN8
B	1235	HIS	-	expression tag	UNP A0A346FJN8
B	1236	HIS	-	expression tag	UNP A0A346FJN8
B	1237	HIS	-	expression tag	UNP A0A346FJN8
B	1238	HIS	-	expression tag	UNP A0A346FJN8
B	1239	HIS	-	expression tag	UNP A0A346FJN8
B	1240	HIS	-	expression tag	UNP A0A346FJN8
B	1241	SER	-	expression tag	UNP A0A346FJN8
B	1242	ALA	-	expression tag	UNP A0A346FJN8
B	1243	TRP	-	expression tag	UNP A0A346FJN8
B	1244	SER	-	expression tag	UNP A0A346FJN8
B	1245	HIS	-	expression tag	UNP A0A346FJN8
B	1246	PRO	-	expression tag	UNP A0A346FJN8
B	1247	GLN	-	expression tag	UNP A0A346FJN8
B	1248	PHE	-	expression tag	UNP A0A346FJN8
B	1249	GLU	-	expression tag	UNP A0A346FJN8
B	1250	LYS	-	expression tag	UNP A0A346FJN8
B	1251	GLY	-	expression tag	UNP A0A346FJN8
B	1252	GLY	-	expression tag	UNP A0A346FJN8
B	1253	GLY	-	expression tag	UNP A0A346FJN8
B	1254	SER	-	expression tag	UNP A0A346FJN8
B	1255	GLY	-	expression tag	UNP A0A346FJN8
B	1256	GLY	-	expression tag	UNP A0A346FJN8
B	1257	GLY	-	expression tag	UNP A0A346FJN8
B	1258	GLY	-	expression tag	UNP A0A346FJN8
B	1259	SER	-	expression tag	UNP A0A346FJN8
B	1260	GLY	-	expression tag	UNP A0A346FJN8
B	1261	GLY	-	expression tag	UNP A0A346FJN8
B	1262	SER	-	expression tag	UNP A0A346FJN8
B	1263	ALA	-	expression tag	UNP A0A346FJN8
B	1264	TRP	-	expression tag	UNP A0A346FJN8
B	1265	SER	-	expression tag	UNP A0A346FJN8
B	1266	HIS	-	expression tag	UNP A0A346FJN8
B	1267	PRO	-	expression tag	UNP A0A346FJN8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1268	GLN	-	expression tag	UNP A0A346FJN8
B	1269	PHE	-	expression tag	UNP A0A346FJN8
B	1270	GLU	-	expression tag	UNP A0A346FJN8
B	1271	LYS	-	expression tag	UNP A0A346FJN8
C	969	PRO	LYS	conflict	UNP U5WI05
C	970	PRO	VAL	conflict	UNP U5WI05
C	1192	GLY	-	linker	UNP U5WI05
C	1193	SER	-	linker	UNP U5WI05
C	1220	LEU	-	expression tag	UNP A0A346FJN8
C	1221	GLY	-	expression tag	UNP A0A346FJN8
C	1222	ARG	-	expression tag	UNP A0A346FJN8
C	1223	SER	-	expression tag	UNP A0A346FJN8
C	1224	LEU	-	expression tag	UNP A0A346FJN8
C	1225	GLU	-	expression tag	UNP A0A346FJN8
C	1226	VAL	-	expression tag	UNP A0A346FJN8
C	1227	LEU	-	expression tag	UNP A0A346FJN8
C	1228	PHE	-	expression tag	UNP A0A346FJN8
C	1229	GLN	-	expression tag	UNP A0A346FJN8
C	1230	GLY	-	expression tag	UNP A0A346FJN8
C	1231	PRO	-	expression tag	UNP A0A346FJN8
C	1232	GLY	-	expression tag	UNP A0A346FJN8
C	1233	HIS	-	expression tag	UNP A0A346FJN8
C	1234	HIS	-	expression tag	UNP A0A346FJN8
C	1235	HIS	-	expression tag	UNP A0A346FJN8
C	1236	HIS	-	expression tag	UNP A0A346FJN8
C	1237	HIS	-	expression tag	UNP A0A346FJN8
C	1238	HIS	-	expression tag	UNP A0A346FJN8
C	1239	HIS	-	expression tag	UNP A0A346FJN8
C	1240	HIS	-	expression tag	UNP A0A346FJN8
C	1241	SER	-	expression tag	UNP A0A346FJN8
C	1242	ALA	-	expression tag	UNP A0A346FJN8
C	1243	TRP	-	expression tag	UNP A0A346FJN8
C	1244	SER	-	expression tag	UNP A0A346FJN8
C	1245	HIS	-	expression tag	UNP A0A346FJN8
C	1246	PRO	-	expression tag	UNP A0A346FJN8
C	1247	GLN	-	expression tag	UNP A0A346FJN8
C	1248	PHE	-	expression tag	UNP A0A346FJN8
C	1249	GLU	-	expression tag	UNP A0A346FJN8
C	1250	LYS	-	expression tag	UNP A0A346FJN8
C	1251	GLY	-	expression tag	UNP A0A346FJN8
C	1252	GLY	-	expression tag	UNP A0A346FJN8
C	1253	GLY	-	expression tag	UNP A0A346FJN8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1254	SER	-	expression tag	UNP A0A346FJN8
C	1255	GLY	-	expression tag	UNP A0A346FJN8
C	1256	GLY	-	expression tag	UNP A0A346FJN8
C	1257	GLY	-	expression tag	UNP A0A346FJN8
C	1258	GLY	-	expression tag	UNP A0A346FJN8
C	1259	SER	-	expression tag	UNP A0A346FJN8
C	1260	GLY	-	expression tag	UNP A0A346FJN8
C	1261	GLY	-	expression tag	UNP A0A346FJN8
C	1262	SER	-	expression tag	UNP A0A346FJN8
C	1263	ALA	-	expression tag	UNP A0A346FJN8
C	1264	TRP	-	expression tag	UNP A0A346FJN8
C	1265	SER	-	expression tag	UNP A0A346FJN8
C	1266	HIS	-	expression tag	UNP A0A346FJN8
C	1267	PRO	-	expression tag	UNP A0A346FJN8
C	1268	GLN	-	expression tag	UNP A0A346FJN8
C	1269	PHE	-	expression tag	UNP A0A346FJN8
C	1270	GLU	-	expression tag	UNP A0A346FJN8
C	1271	LYS	-	expression tag	UNP A0A346FJN8

- 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		

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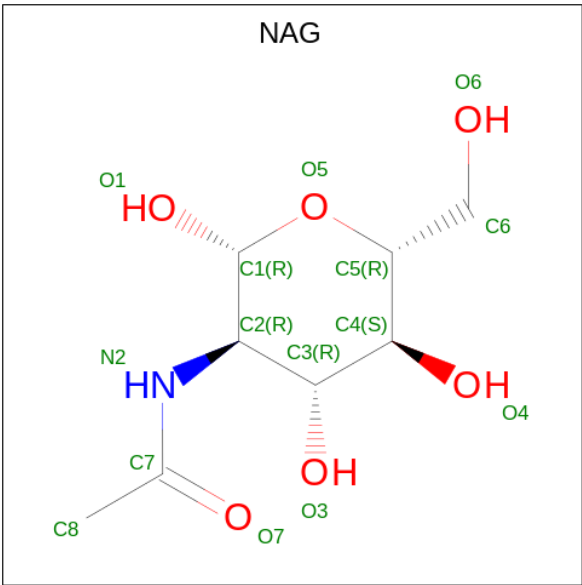
Mol	Chain	Residues	Atoms				AltConf	Trace
2	M	2	Total	C	N	O	0	0
			28	16	2	10		
2	N	2	Total	C	N	O	0	0
			28	16	2	10		
2	O	2	Total	C	N	O	0	0
			28	16	2	10		
2	P	2	Total	C	N	O	0	0
			28	16	2	10		
2	R	2	Total	C	N	O	0	0
			28	16	2	10		
2	S	2	Total	C	N	O	0	0
			28	16	2	10		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
3	K	3	Total	C	N	O	0	0
			39	22	2	15		
3	L	3	Total	C	N	O	0	0
			39	22	2	15		
3	Q	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				AltConf
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	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	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	

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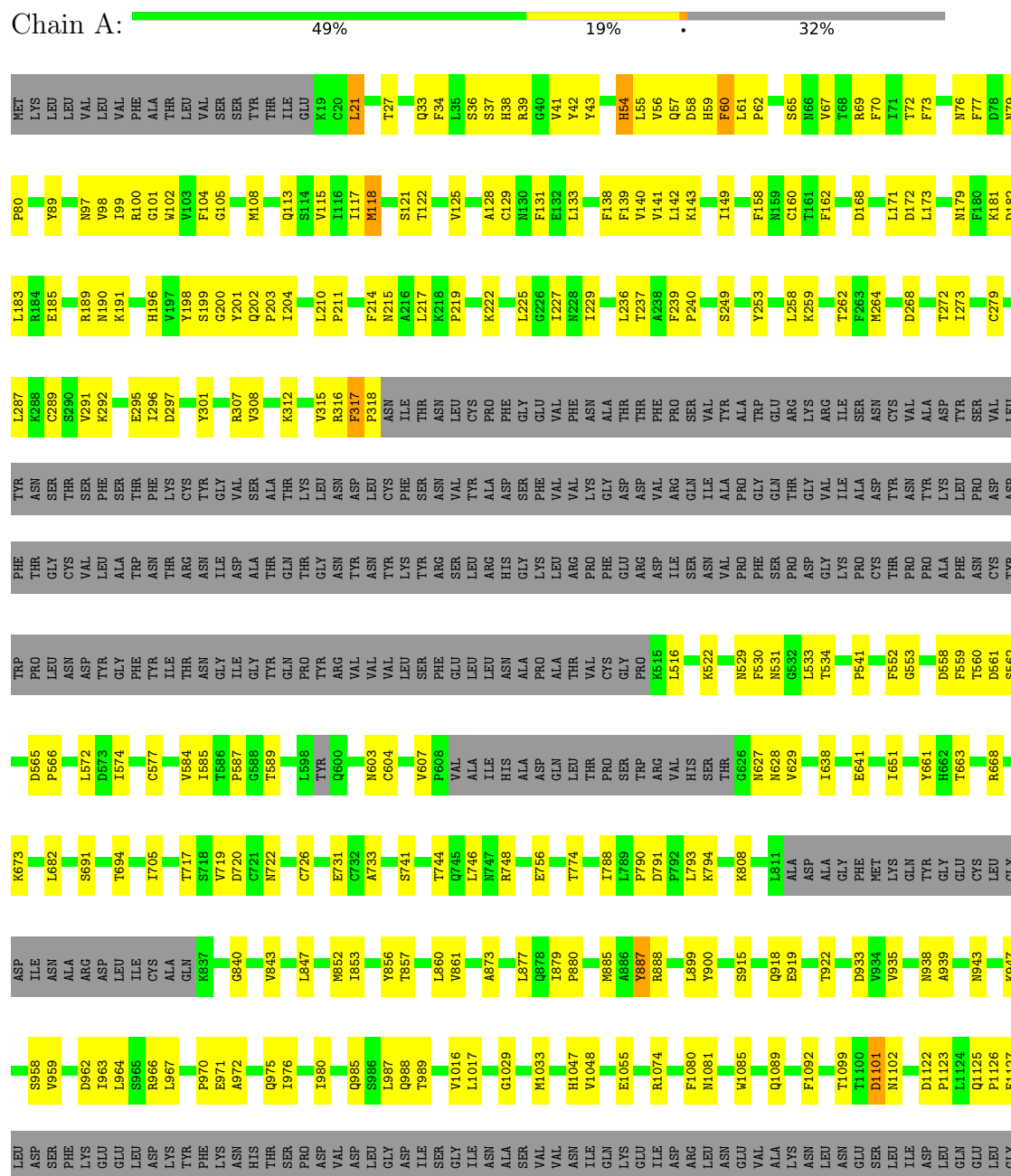
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Mol	Chain	Residues	Atoms				AltConf
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	

### 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







Chain E:  50% 50%



- 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:  50% 50%



- 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:  50% 50%



- 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:  50% 50%



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

Chain O:  50% 50%



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

Chain P:  100%



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

Chain R:  50% 50%



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

Chain S:  100%



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

Chain K:  100%



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

Chain L:  100%





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

Chain Q:  33% 67%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	59319	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.29	0/6907	0.51	0/9391
1	B	0.29	0/8527	0.52	0/11611
1	C	0.29	0/6921	0.52	1/9412 (0.0%)
All	All	0.29	0/22355	0.52	1/30414 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	119	ASN	N-CA-C	-5.48	96.21	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6757	0	6607	180	0
1	B	8325	0	8085	192	0
1	C	6769	0	6611	155	0
2	D	28	0	25	0	0
2	E	28	0	25	1	0
2	F	28	0	25	1	0
2	G	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	28	0	25	0	0
2	I	28	0	25	1	0
2	J	28	0	25	0	0
2	M	28	0	25	0	0
2	N	28	0	25	1	0
2	O	28	0	25	1	0
2	P	28	0	25	0	0
2	R	28	0	25	1	0
2	S	28	0	25	0	0
3	K	39	0	34	0	0
3	L	39	0	34	0	0
3	Q	39	0	34	1	0
4	A	56	0	52	1	0
4	B	84	0	78	0	0
4	C	126	0	117	2	0
All	All	22598	0	21977	503	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 11.

All (503) 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:128:ALA:HB3	1:A:162:PHE:HB3	1.52	0.90
1:A:315:VAL:HG23	1:A:529:ASN:HB3	1.55	0.86
1:A:69:ARG:HH22	1:A:210:LEU:HB2	1.46	0.80
1:A:1099:THR:HG22	1:A:1101:ASP:H	1.47	0.80
1:A:852:MET:HG2	1:C:682:LEU:HD21	1.65	0.78
1:C:81:ILE:HD11	1:C:231:ASN:HB2	1.67	0.76
1:C:598:LEU:HD11	1:C:653:ILE:HG23	1.67	0.76
1:A:104:PHE:HB2	1:A:115:VAL:HG22	1.69	0.75
1:B:663:THR:HA	1:B:673:LYS:HA	1.68	0.75
1:C:27:THR:HB	1:C:76:ASN:HB3	1.69	0.75
1:C:599:TYR:O	1:C:635:GLY:HA3	1.87	0.74
1:A:629:VAL:HG13	1:A:638:ILE:HG13	1.70	0.74
1:A:36:SER:HB3	1:A:65:SER:H	1.53	0.74
1:B:377:ASP:HA	1:B:515:LYS:HD2	1.70	0.74
1:C:39:ARG:HH22	1:C:202:GLN:HE22	1.37	0.73
1:C:522:LYS:HD3	1:C:541:PRO:HD3	1.71	0.72
1:A:104:PHE:HB3	1:A:229:ILE:HG21	1.71	0.72
1:B:129:CYS:SG	1:B:160:CYS:N	2.63	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:ALA:HB3	1:B:162:PHE:HB3	1.73	0.71
1:B:264:MET:HB3	1:B:277:VAL:HG22	1.72	0.71
1:A:959:VAL:HG12	1:A:962:ASP:H	1.55	0.70
1:A:105:GLY:HA3	1:A:108:MET:HE1	1.74	0.70
1:B:79:ASN:O	1:B:233:ARG:NH2	2.26	0.68
1:B:404:GLY:O	1:B:408:ASP:N	2.25	0.68
1:B:326:PHE:HB3	1:B:330:PHE:CE2	2.29	0.67
1:C:115:VAL:HG21	1:C:225:LEU:HD13	1.75	0.67
1:A:69:ARG:NH2	1:A:210:LEU:HB2	2.10	0.67
1:B:391:LYS:HE3	1:B:393:ASP:HB2	1.77	0.66
1:C:774:THR:HG23	1:C:789:LEU:HD22	1.77	0.66
1:B:194:PHE:CE2	1:B:222:LYS:HG2	2.31	0.65
1:B:117:ILE:HG23	1:B:126:ILE:HG12	1.79	0.65
1:A:189:ARG:NH2	1:A:190:ASN:O	2.29	0.65
1:C:32:THR:HG23	1:C:69:ARG:HB3	1.78	0.65
1:B:98:VAL:HG13	1:B:237:THR:HG22	1.79	0.65
1:A:77:PHE:HE1	1:A:79:ASN:HB2	1.62	0.64
1:B:326:PHE:HB3	1:B:330:PHE:HE2	1.62	0.64
1:B:705:ILE:HD12	1:B:1048:VAL:HG22	1.79	0.64
1:C:746:LEU:HD22	1:C:991:VAL:HG21	1.79	0.64
1:A:1029:GLY:HA2	1:B:873:ALA:HB1	1.80	0.64
1:A:561:ASP:O	1:A:574:ILE:N	2.28	0.63
1:C:298:LYS:HG2	1:C:651:ILE:HD11	1.80	0.63
1:B:122:THR:O	1:B:169:PHE:N	2.32	0.63
1:C:195:LEU:HD12	1:C:225:LEU:HD12	1.80	0.63
1:A:682:LEU:HD11	1:B:852:MET:HB3	1.80	0.63
1:B:103:VAL:HB	1:B:233:ARG:HG2	1.80	0.63
1:C:975:GLN:OE1	1:C:978:ARG:NH2	2.32	0.62
1:B:972:ALA:O	1:B:976:ILE:HG13	2.00	0.62
1:C:314:VAL:HB	1:C:316:ARG:HH12	1.64	0.62
1:C:794:LYS:NZ	1:C:798:ARG:O	2.32	0.62
1:A:122:THR:HB	1:A:168:ASP:HB3	1.82	0.62
1:A:533:LEU:HD11	1:A:560:THR:HG21	1.81	0.62
1:C:62:PRO:HG2	1:C:259:LYS:HD3	1.81	0.62
1:C:709:VAL:HG22	1:C:1044:VAL:HG22	1.81	0.62
1:A:585:ILE:HG23	1:A:651:ILE:HG21	1.80	0.61
1:A:879:ILE:HG13	1:C:695:ILE:HD13	1.82	0.61
1:B:430:ASP:OD1	1:B:496:ARG:NH2	2.34	0.61
1:C:307:ARG:HH11	1:C:579:PHE:HB3	1.64	0.61
1:C:24:ASP:H	1:C:246:TRP:HZ3	1.45	0.61
1:B:103:VAL:HG23	1:B:235:LEU:HD11	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1074:ARG:HG2	1:B:1075:GLU:HG2	1.83	0.61
1:C:29:PRO:HG3	1:C:78:ASP:HB3	1.81	0.61
1:B:440:LYS:HG2	1:B:481:ASP:HB3	1.83	0.60
1:C:304:SER:OG	1:C:305:ASN:N	2.34	0.60
1:A:717:THR:HG22	1:A:843:VAL:HG22	1.82	0.60
1:B:76:ASN:ND2	1:B:78:ASP:OD2	2.34	0.60
1:B:363:SER:N	1:B:423:ALA:O	2.34	0.60
1:B:969:PRO:HG2	1:B:970:PRO:HD3	1.83	0.60
1:C:1105:VAL:HG23	1:C:1106:SER:H	1.67	0.60
1:B:421:VAL:HG22	1:B:499:VAL:HG22	1.82	0.59
1:B:21:LEU:HB2	1:B:138:PHE:HZ	1.68	0.59
1:A:915:SER:O	1:A:919:GLU:HG2	2.03	0.58
1:B:477:TRP:HE3	1:B:478:PRO:HD2	1.68	0.58
1:B:204:ILE:HG21	1:B:211:PRO:HG3	1.85	0.58
1:A:115:VAL:HG11	1:A:225:LEU:HD13	1.85	0.58
1:C:641:GLU:OE2	1:C:641:GLU:N	2.35	0.58
1:A:101:GLY:HA3	1:A:117:ILE:O	2.04	0.58
1:C:87:GLY:HA2	1:C:188:PHE:O	2.03	0.58
1:C:265:LEU:HD23	1:C:273:ILE:HD13	1.85	0.58
1:A:34:PHE:HD1	1:A:69:ARG:HG3	1.69	0.57
1:A:307:ARG:HE	1:A:308:VAL:H	1.49	0.57
1:B:225:LEU:HB3	1:B:227:ILE:HG12	1.86	0.57
1:B:448:LYS:HB3	1:B:448:LYS:HZ2	1.68	0.57
1:A:236:LEU:HD11	1:A:253:TYR:CE1	2.39	0.57
1:C:202:GLN:OE1	1:C:215:ASN:ND2	2.37	0.57
1:A:972:ALA:O	1:A:976:ILE:HG12	2.03	0.57
1:C:316:ARG:NH1	1:C:519:ASP:O	2.37	0.57
1:C:59:HIS:CE1	1:C:260:PRO:HB3	2.39	0.57
1:A:100:ARG:HH21	1:A:141:VAL:HG21	1.70	0.57
1:B:914:ILE:O	1:B:917:ILE:HG22	2.03	0.57
1:A:34:PHE:HB2	1:A:69:ARG:NE	2.20	0.57
1:A:97:ASN:ND2	1:A:172:ASP:O	2.35	0.57
1:A:196:HIS:HB3	1:A:198:TYR:HE1	1.70	0.57
1:A:287:LEU:HD12	1:A:584:VAL:HB	1.86	0.56
1:A:726:CYS:SG	1:A:733:ALA:N	2.78	0.56
2:F:2:NAG:H3	2:F:2:NAG:H83	1.85	0.56
1:A:36:SER:HB2	1:A:67:VAL:HG21	1.86	0.56
1:A:55:LEU:HD12	1:A:264:MET:HG2	1.87	0.56
1:A:57:GLN:HG2	1:A:262:THR:HG22	1.86	0.56
1:A:985:GLN:O	1:A:989:THR:HG23	2.05	0.56
1:B:101:GLY:HA3	1:B:117:ILE:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:194:PHE:HE2	1:B:222:LYS:HG2	1.70	0.56
1:A:853:ILE:O	1:A:857:THR:HG23	2.04	0.56
1:B:103:VAL:HG22	1:B:116:ILE:HG12	1.88	0.56
1:A:880:PRO:HA	1:C:690:TYR:HE1	1.69	0.56
1:A:295:GLU:HA	1:A:589:THR:HG21	1.87	0.56
1:C:888:ARG:O	1:C:892:ILE:HD12	2.05	0.56
1:B:132:GLU:OE2	1:B:155:ASN:ND2	2.33	0.56
1:C:1074:ARG:NH2	1:C:1101:ASP:O	2.35	0.56
1:A:129:CYS:SG	1:A:160:CYS:N	2.78	0.56
1:A:198:TYR:CE2	1:A:219:PRO:HB3	2.41	0.56
1:B:341:TRP:CZ3	1:B:343:ARG:HB2	2.40	0.56
1:A:746:LEU:HD21	1:A:988:GLN:HG2	1.88	0.55
1:B:140:VAL:HB	1:B:149:ILE:HB	1.87	0.55
1:A:138:PHE:CE2	1:A:140:VAL:HG22	2.41	0.55
1:B:199:SER:HB3	1:B:220:ILE:HG21	1.88	0.55
1:B:793:LEU:HB2	1:B:794:LYS:NZ	2.21	0.55
1:A:287:LEU:HD11	1:A:301:TYR:HD2	1.71	0.55
1:A:791:ASP:HB2	1:A:794:LYS:HD2	1.88	0.55
1:B:477:TRP:CE3	1:B:478:PRO:HD2	2.42	0.55
1:A:530:PHE:HE1	1:A:572:LEU:HD12	1.71	0.55
1:A:705:ILE:HA	1:A:1047:HIS:O	2.07	0.55
1:B:27:THR:O	1:B:76:ASN:ND2	2.39	0.55
1:B:1059:THR:HB	1:B:1080:PHE:HB3	1.88	0.55
1:B:1104:PHE:HE2	1:C:897:ASN:HD21	1.55	0.55
1:B:1036:PRO:O	1:B:1037:GLN:NE2	2.30	0.55
1:C:718:SER:OG	1:C:842:THR:OG1	2.22	0.55
1:A:113:GLN:HB2	1:A:227:ILE:HG21	1.88	0.55
1:A:98:VAL:HA	1:A:237:THR:HG22	1.89	0.55
1:B:180:PHE:HB2	1:B:206:ALA:HB3	1.88	0.54
1:B:791:ASP:HB2	1:B:794:LYS:HG2	1.88	0.54
1:B:915:SER:O	1:B:919:GLU:HG3	2.07	0.54
1:B:137:PRO:HB3	1:B:153:ILE:HG23	1.90	0.54
1:B:400:PRO:HB3	1:B:415:ASP:HA	1.90	0.54
1:A:262:THR:OG1	1:A:279:CYS:SG	2.65	0.54
1:C:299:GLY:HA2	1:C:651:ILE:HD12	1.88	0.54
1:B:91:ALA:HB1	1:B:183:LEU:HD11	1.89	0.54
1:A:1122:ASP:OD2	1:A:1125:GLN:NE2	2.41	0.54
1:B:117:ILE:HG12	1:B:126:ILE:HG23	1.90	0.54
1:B:381:SER:HB3	1:B:509:ALA:HA	1.91	0.53
1:A:1081:ASN:ND2	2:E:1:NAG:O7	2.42	0.53
1:C:126:ILE:HG12	1:C:164:TYR:HD2	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:802:GLU:HA	1:C:805:LEU:HD12	1.89	0.53
1:B:102:TRP:HD1	1:B:232:PHE:HE1	1.57	0.53
1:A:552:PHE:O	1:B:48:PHE:N	2.25	0.53
1:A:731:GLU:OE2	1:A:964:LEU:HD22	2.09	0.53
1:B:448:LYS:HB3	1:B:448:LYS:NZ	2.23	0.53
1:B:707:THR:HG22	1:B:917:ILE:HD11	1.91	0.53
1:C:805:LEU:O	1:C:809:VAL:HG12	2.09	0.53
1:B:583:SER:OG	1:B:598:LEU:HB3	2.09	0.52
1:C:59:HIS:HB2	1:C:189:ARG:NH1	2.24	0.52
1:C:714:MET:HB2	1:C:938:ASN:HD21	1.74	0.52
1:C:733:ALA:HA	1:C:736:LEU:HB3	1.89	0.52
1:A:522:LYS:NZ	1:A:541:PRO:HG3	2.24	0.52
1:A:663:THR:HA	1:A:673:LYS:HA	1.91	0.52
1:C:200:GLY:HA3	1:C:217:LEU:HD22	1.91	0.52
1:A:553:GLY:N	1:A:562:SER:O	2.42	0.52
1:A:691:SER:HB3	1:A:694:THR:HG22	1.91	0.52
1:C:287:LEU:HD13	1:C:584:VAL:HB	1.90	0.52
1:A:104:PHE:HB3	1:A:229:ILE:HD13	1.91	0.52
1:A:121:SER:HA	1:A:171:LEU:HB3	1.91	0.52
1:A:1016:VAL:HG12	1:A:1017:LEU:HD23	1.92	0.52
1:B:89:TYR:HE1	1:B:185:GLU:HB3	1.75	0.52
1:B:717:THR:HG22	1:B:843:VAL:HG22	1.92	0.52
1:C:269:GLU:OE1	2:O:1:NAG:N2	2.40	0.52
1:C:307:ARG:NH1	1:C:578:SER:O	2.43	0.52
1:C:767:GLN:HG3	1:C:1012:MET:HG2	1.91	0.52
1:A:888:ARG:HD3	1:A:1033:MET:HG2	1.91	0.52
1:C:39:ARG:NH1	1:C:185:GLU:OE2	2.43	0.52
1:C:317:PHE:HE2	1:C:516:LEU:HA	1.74	0.52
1:C:888:ARG:HD3	1:C:1032:LEU:O	2.09	0.52
1:A:663:THR:HB	1:A:673:LYS:HG2	1.91	0.51
1:C:305:ASN:HA	1:C:581:GLY:HA2	1.92	0.51
1:B:948:GLN:HG2	1:B:986:SER:OG	2.10	0.51
1:A:1125:GLN:HG3	1:A:1126:PRO:HD3	1.92	0.51
1:B:426:THR:HG21	1:B:496:ARG:HG3	1.92	0.51
1:B:102:TRP:HD1	1:B:232:PHE:CE1	2.28	0.51
1:A:54:HIS:CE1	1:A:56:VAL:HB	2.45	0.51
1:A:318:PRO:HD3	1:A:531:ASN:HA	1.92	0.51
1:B:1029:GLY:HA2	1:C:873:ALA:HB1	1.92	0.51
1:A:200:GLY:HA3	1:A:217:LEU:HD22	1.92	0.51
1:B:390:VAL:HB	1:B:394:ASP:HB2	1.92	0.51
1:B:1031:HIS:HA	1:B:1049:THR:HG22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:ASP:OD1	1:A:272:THR:N	2.41	0.51
1:B:977:ASP:HA	1:B:980:ILE:HG22	1.92	0.51
1:A:264:MET:SD	1:A:289:CYS:HA	2.51	0.51
1:B:326:PHE:CE1	1:B:346:ILE:HG21	2.46	0.51
1:B:682:LEU:HD21	1:C:852:MET:HG2	1.92	0.51
1:A:1089:GLN:HE21	1:A:1092:PHE:HB3	1.76	0.51
1:B:339:TYR:HE1	1:B:440:LYS:HB2	1.76	0.51
1:B:1090:ARG:NH2	1:C:887:TYR:HB2	2.26	0.51
1:C:718:SER:HB3	1:C:844:LEU:HD11	1.93	0.51
1:C:516:LEU:HG	1:C:517:SER:H	1.76	0.50
1:C:588:GLY:O	1:C:591:THR:N	2.43	0.50
1:A:179:ASN:HB3	1:A:181:LYS:HG2	1.94	0.50
1:C:69:ARG:NH2	1:C:208:SER:O	2.28	0.50
1:B:82:ILE:HD12	1:B:232:PHE:CE2	2.47	0.50
1:C:653:ILE:HD11	1:C:659:ALA:HB2	1.92	0.50
1:A:189:ARG:HH21	1:A:191:LYS:HG3	1.75	0.50
1:C:162:PHE:HE2	1:C:224:PRO:HD2	1.77	0.50
1:C:668:ARG:CD	1:C:669:SER:H	2.25	0.50
1:A:719:VAL:HG11	1:A:987:LEU:HD11	1.93	0.50
1:C:809:VAL:HB	1:C:928:LEU:HD23	1.94	0.50
1:A:918:GLN:O	1:A:922:THR:OG1	2.21	0.50
1:A:34:PHE:H	1:A:69:ARG:HD3	1.76	0.50
1:B:351:ALA:O	1:B:514:PRO:HD3	2.11	0.50
1:C:314:VAL:HG23	1:C:528:PHE:HA	1.94	0.50
1:A:104:PHE:HB2	1:A:115:VAL:CG2	2.40	0.50
1:A:118:MET:HB3	1:A:139:PHE:HZ	1.77	0.50
1:B:346:ILE:HB	1:B:383:VAL:HG13	1.94	0.50
1:B:682:LEU:HB3	1:C:856:TYR:CZ	2.47	0.50
1:B:968:ASP:OD1	1:B:969:PRO:HD2	2.12	0.50
1:B:1073:PRO:HD3	1:B:1078:PHE:CE2	2.47	0.50
1:A:59:HIS:O	1:A:258:LEU:HD12	2.12	0.49
1:C:246:TRP:CD1	1:C:246:TRP:N	2.80	0.49
1:C:599:TYR:HB3	1:C:602:VAL:HG22	1.93	0.49
1:B:210:LEU:HD12	1:B:211:PRO:HD2	1.94	0.49
1:B:885:MET:HG3	1:B:899:LEU:HD11	1.94	0.49
1:A:27:THR:N	1:A:76:ASN:OD1	2.45	0.49
1:B:326:PHE:HE1	1:B:346:ILE:HG21	1.77	0.49
1:B:332:ALA:HB3	1:B:335:PHE:CE1	2.47	0.49
1:C:239:PHE:N	1:C:247:GLY:O	2.44	0.49
1:C:791:ASP:HB2	1:C:794:LYS:HG2	1.94	0.49
1:A:99:ILE:CD1	1:A:253:TYR:HB3	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:VAL:HG12	1:A:128:ALA:HB2	1.94	0.49
1:B:269:GLU:HB3	2:N:1:NAG:H82	1.94	0.49
1:B:301:TYR:O	1:B:584:VAL:N	2.35	0.49
1:B:397:GLN:HE21	1:B:407:ALA:HB2	1.77	0.49
1:C:563:VAL:HB	1:C:574:ILE:HD11	1.94	0.49
1:C:287:LEU:HD11	1:C:301:TYR:HB3	1.95	0.49
1:A:115:VAL:HA	1:A:128:ALA:HA	1.94	0.49
1:A:129:CYS:HA	1:A:160:CYS:HA	1.94	0.49
1:A:1080:PHE:HB2	1:A:1085:TRP:CZ3	2.48	0.49
1:B:579:PHE:HB2	1:C:838:PHE:CZ	2.48	0.49
1:B:389:VAL:HG22	1:B:496:ARG:HG2	1.95	0.49
1:C:181:LYS:HA	1:C:205:SER:HB3	1.94	0.49
1:C:886:ALA:HB2	1:C:899:LEU:HD22	1.95	0.49
1:C:284:LEU:HB2	1:C:595:VAL:HG11	1.94	0.49
1:A:287:LEU:HD11	1:A:301:TYR:CD2	2.46	0.48
1:B:409:TYR:CD2	1:B:445:ARG:HB3	2.48	0.48
1:B:1087:ILE:HG21	1:B:1102:ASN:HB3	1.94	0.48
1:C:51:ASN:N	1:C:267:TYR:O	2.46	0.48
1:C:51:ASN:CA	1:C:267:TYR:O	2.61	0.48
1:C:312:LYS:HD3	1:C:521:ILE:HG13	1.96	0.48
1:A:202:GLN:OE1	1:A:215:ASN:ND2	2.46	0.48
1:B:100:ARG:HB2	1:B:139:PHE:HE2	1.78	0.48
1:B:102:TRP:CD1	1:B:232:PHE:HE1	2.31	0.48
1:C:129:CYS:HB3	1:C:131:PHE:CE2	2.48	0.48
1:A:308:VAL:HB	1:A:577:CYS:SG	2.54	0.48
1:A:628:ASN:ND2	1:A:641:GLU:HG3	2.27	0.48
1:B:736:LEU:HG	1:B:980:ILE:HD11	1.96	0.48
1:B:960:LEU:HD23	1:B:960:LEU:H	1.78	0.48
1:C:142:LEU:HD21	1:C:149:ILE:CD1	2.44	0.48
1:C:156:ASN:OD1	1:C:156:ASN:N	2.46	0.48
1:C:709:VAL:O	1:C:930:LYS:NZ	2.30	0.48
1:A:185:GLU:O	1:A:199:SER:HA	2.13	0.48
1:C:977:ASP:OD1	1:C:978:ARG:N	2.47	0.48
1:B:26:ARG:HD2	1:B:77:PHE:HD2	1.78	0.48
1:C:522:LYS:HB2	1:C:522:LYS:HE2	1.53	0.48
1:B:187:VAL:O	1:B:197:VAL:HA	2.14	0.47
1:A:559:PHE:HZ	1:B:946:VAL:HG11	1.79	0.47
1:B:890:ASN:HD22	1:B:890:ASN:HA	1.51	0.47
1:B:698:PRO:HA	1:B:1055:GLU:HA	1.95	0.47
1:A:100:ARG:HH22	1:A:173:LEU:HB3	1.80	0.47
1:C:561:ASP:O	1:C:574:ILE:N	2.36	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:698:PRO:HA	1:C:1055:GLU:HA	1.96	0.47
1:A:522:LYS:HD3	1:A:541:PRO:HD3	1.97	0.47
1:A:21:LEU:HD23	1:A:21:LEU:H	1.80	0.47
1:A:970:PRO:HB2	1:A:971:GLU:OE2	2.15	0.47
1:B:317:PHE:O	1:B:567:LYS:HD3	2.14	0.47
1:B:450:ARG:HB2	1:B:453:GLU:HG3	1.97	0.47
1:A:108:MET:SD	1:A:133:LEU:HG	2.55	0.47
1:C:51:ASN:HA	1:C:267:TYR:O	2.15	0.47
1:C:70:PHE:HB2	1:C:253:TYR:CZ	2.50	0.47
1:C:1066:HIS:CD2	1:C:1067:GLU:HB2	2.50	0.47
1:A:72:THR:O	1:A:72:THR:HG23	2.14	0.47
1:B:661:TYR:HD1	1:B:675:ILE:HG12	1.80	0.47
1:C:627:ASN:OD1	1:C:627:ASN:N	2.48	0.47
1:C:958:SER:O	1:C:958:SER:OG	2.32	0.47
1:B:27:THR:HB	1:B:76:ASN:HA	1.97	0.47
1:A:847:LEU:HD12	1:C:654:GLY:HA2	1.97	0.47
1:B:330:PHE:CD1	1:B:498:VAL:HG21	2.50	0.47
1:B:332:ALA:HB3	1:B:335:PHE:HE1	1.80	0.47
1:A:316:ARG:NH1	1:A:565:ASP:OD1	2.49	0.46
1:B:554:ARG:HG3	1:C:47:ILE:HG21	1.97	0.46
1:C:668:ARG:HD3	1:C:669:SER:H	1.80	0.46
1:C:905:GLN:O	1:C:909:GLN:HG3	2.16	0.46
1:A:316:ARG:HG2	1:A:566:PRO:HG2	1.97	0.46
1:B:105:GLY:O	1:B:231:ASN:HB3	2.16	0.46
1:B:587:PRO:HG3	1:B:661:TYR:CD1	2.49	0.46
1:B:957:SER:O	1:B:963:ILE:HD11	2.15	0.46
1:A:307:ARG:HD2	1:A:307:ARG:HA	1.72	0.46
1:A:963:ILE:HD13	1:A:975:GLN:HB3	1.97	0.46
1:C:892:ILE:HD12	1:C:892:ILE:H	1.80	0.46
1:A:774:THR:HG21	1:A:790:PRO:HG2	1.97	0.46
1:A:880:PRO:HA	1:C:690:TYR:CE1	2.49	0.46
1:A:1099:THR:HG23	1:A:1123:PRO:HD3	1.97	0.46
1:B:601:ASP:OD1	1:C:842:THR:HG21	2.15	0.46
1:A:705:ILE:HG12	1:A:1048:VAL:HG22	1.97	0.46
1:B:174:GLY:HA2	1:B:239:PHE:HE2	1.81	0.46
1:B:808:LYS:HA	1:B:808:LYS:HD3	1.68	0.46
1:C:653:ILE:HB	1:C:657:ILE:HG13	1.96	0.46
1:A:183:LEU:HB2	1:A:202:GLN:HB2	1.98	0.46
1:B:127:ARG:HD2	1:B:160:CYS:SG	2.55	0.46
1:B:455:ASP:OD1	1:B:455:ASP:N	2.49	0.46
1:B:287:LEU:HD22	1:B:296:ILE:HG13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:ILE:HG23	1:A:211:PRO:HG2	1.98	0.45
1:A:296:ILE:HD13	1:A:296:ILE:HA	1.83	0.45
1:A:587:PRO:HG3	1:A:661:TYR:CD1	2.51	0.45
1:C:969:PRO:HA	1:C:972:ALA:HB3	1.96	0.45
1:C:142:LEU:HD21	1:C:149:ILE:HG12	1.99	0.45
1:C:808:LYS:HZ3	1:C:924:THR:HA	1.82	0.45
1:A:118:MET:SD	1:A:118:MET:N	2.89	0.45
1:B:386:ASP:OD2	1:B:411:TYR:OH	2.33	0.45
1:A:264:MET:HE1	1:A:292:LYS:HA	1.99	0.45
1:A:857:THR:O	1:A:861:VAL:HG23	2.17	0.45
1:C:1083:THR:HG21	2:R:1:NAG:H3	1.99	0.45
1:A:887:TYR:HB2	1:C:1090:ARG:NH2	2.31	0.45
1:B:120:ASN:HB3	1:B:123:ASN:O	2.16	0.45
1:B:140:VAL:HG23	1:B:151:SER:HB3	1.98	0.45
1:B:92:ALA:O	1:B:183:LEU:HA	2.17	0.45
2:I:1:NAG:H61	2:I:2:NAG:HN2	1.82	0.45
1:A:529:ASN:ND2	1:A:534:THR:OG1	2.50	0.45
1:A:793:LEU:H	1:A:793:LEU:HD23	1.81	0.45
1:B:319:ASN:H	1:B:567:LYS:HZ1	1.64	0.45
1:B:977:ASP:O	1:B:980:ILE:HG22	2.16	0.45
1:B:1080:PHE:HB2	1:B:1085:TRP:CZ3	2.51	0.45
1:C:73:PHE:HA	1:C:250:ALA:HA	1.99	0.45
1:B:140:VAL:HG12	1:B:149:ILE:HD12	1.99	0.45
1:B:462:SER:HB2	1:B:468:CYS:SG	2.57	0.45
1:B:525:CYS:HB2	1:B:577:CYS:HB3	1.84	0.45
1:A:143:LYS:HD3	1:A:239:PHE:HB3	1.99	0.45
1:A:287:LEU:O	1:A:291:VAL:HG23	2.17	0.45
1:A:885:MET:HB3	1:A:899:LEU:HD11	1.99	0.45
1:B:533:LEU:HD12	1:B:533:LEU:HA	1.77	0.45
1:C:562:SER:HA	1:C:572:LEU:O	2.17	0.45
1:A:142:LEU:HA	1:A:240:PRO:HD2	1.98	0.44
1:A:222:LYS:HB2	1:A:222:LYS:HE3	1.81	0.44
1:A:317:PHE:CD2	1:A:318:PRO:HD2	2.52	0.44
1:A:852:MET:CG	1:C:682:LEU:HD21	2.42	0.44
1:B:579:PHE:HB2	1:C:838:PHE:CE1	2.52	0.44
1:C:121:SER:HB3	4:C:1309:NAG:H82	1.99	0.44
1:B:461:PHE:N	1:B:478:PRO:HD3	2.33	0.44
1:A:42:TYR:HB2	1:A:198:TYR:CD2	2.53	0.44
1:A:962:ASP:OD1	1:A:966:ARG:HD2	2.18	0.44
1:C:977:ASP:O	1:C:981:THR:HG23	2.18	0.44
1:B:93:THR:HB	1:B:180:PHE:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:316:ARG:NH2	1:B:520:LEU:HB2	2.32	0.44
1:B:955:ALA:HA	1:B:975:GLN:OE1	2.18	0.44
1:A:99:ILE:HD11	1:A:253:TYR:HB3	2.00	0.44
1:A:808:LYS:HA	1:A:808:LYS:HD3	1.79	0.44
1:B:43:TYR:OH	1:B:271:GLY:O	2.28	0.44
1:B:70:PHE:HB2	1:B:253:TYR:CZ	2.52	0.44
1:B:295:GLU:HA	1:B:589:THR:HG21	2.00	0.44
1:B:565:ASP:HB3	1:B:568:THR:O	2.18	0.44
1:C:87:GLY:CA	1:C:188:PHE:O	2.65	0.44
1:A:198:TYR:CZ	1:A:219:PRO:HB3	2.51	0.44
1:C:568:THR:HG22	1:C:569:SER:N	2.33	0.44
1:A:935:VAL:O	1:A:938:ASN:HB3	2.17	0.44
1:B:49:ARG:HB3	1:B:52:VAL:CG2	2.48	0.44
1:B:631:GLN:NE2	1:B:632:THR:O	2.51	0.44
1:C:904:LYS:HE2	1:C:908:ASN:ND2	2.32	0.44
1:B:335:PHE:CE2	1:B:496:ARG:HD3	2.53	0.43
1:A:312:LYS:HE3	1:A:312:LYS:HB2	1.80	0.43
1:B:262:THR:HG23	1:B:279:CYS:SG	2.58	0.43
1:B:759:ARG:NH2	1:B:763:GLU:OE1	2.51	0.43
1:C:520:LEU:O	1:C:521:ILE:HD13	2.18	0.43
1:A:522:LYS:HZ3	1:A:541:PRO:HG3	1.83	0.43
1:B:753:ILE:O	1:B:757:GLN:HG2	2.17	0.43
1:A:976:ILE:O	1:A:980:ILE:HD12	2.18	0.43
1:B:19:LYS:HA	1:B:19:LYS:HD3	1.79	0.43
1:A:70:PHE:CE2	1:A:80:PRO:HG2	2.53	0.43
1:A:791:ASP:HB3	1:A:793:LEU:HD23	2.00	0.43
1:B:21:LEU:HB2	1:B:138:PHE:CZ	2.51	0.43
1:B:179:ASN:O	1:B:181:LYS:N	2.51	0.43
1:A:115:VAL:HG12	1:A:128:ALA:CB	2.49	0.43
1:A:741:SER:HB3	1:A:744:THR:HG22	2.00	0.43
1:A:1055:GLU:H	1:A:1055:GLU:HG2	1.55	0.43
1:B:32:THR:OG1	1:B:69:ARG:HB3	2.18	0.43
1:B:184:ARG:HB3	1:B:186:PHE:HE1	1.83	0.43
1:B:479:LEU:HD13	1:B:479:LEU:HA	1.90	0.43
1:A:873:ALA:HB1	1:C:1029:GLY:HA2	1.99	0.43
1:C:701:PHE:HE2	1:C:906:ILE:HG22	1.83	0.43
1:C:705:ILE:HA	1:C:1047:HIS:O	2.18	0.43
1:B:85:LYS:HB2	1:B:85:LYS:HE2	1.82	0.43
1:B:470:PRO:N	1:B:471:PRO:HD2	2.33	0.43
1:B:653:ILE:HD13	1:B:653:ILE:HA	1.79	0.43
1:B:1012:MET:O	1:B:1016:VAL:HB	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1123:PRO:O	1:B:1126:PRO:HD2	2.19	0.43
1:A:857:THR:HA	1:A:860:LEU:HD12	2.01	0.43
1:A:947:LYS:HD3	1:A:947:LYS:N	2.33	0.43
1:B:127:ARG:NH2	1:B:163:GLU:OE2	2.52	0.43
1:B:885:MET:CG	1:B:899:LEU:HD11	2.48	0.43
1:B:705:ILE:HG12	1:B:913:ALA:HB1	2.01	0.43
1:C:540:THR:O	1:C:573:ASP:N	2.52	0.43
1:A:58:ASP:HB3	1:A:60:PHE:CZ	2.54	0.42
1:B:316:ARG:HA	1:B:316:ARG:HD3	1.80	0.42
1:B:344:LYS:HE2	1:B:345:ARG:O	2.19	0.42
1:B:461:PHE:H	1:B:478:PRO:HD3	1.83	0.42
1:C:126:ILE:O	1:C:126:ILE:HG13	2.19	0.42
1:A:42:TYR:HB2	1:A:198:TYR:HD2	1.83	0.42
1:B:339:TYR:CE1	1:B:440:LYS:HB2	2.54	0.42
1:B:489:GLY:O	1:B:493:GLN:N	2.50	0.42
1:B:799:SER:HB2	1:B:802:GLU:HG3	2.02	0.42
1:B:963:ILE:O	1:B:967:LEU:HB2	2.18	0.42
1:A:118:MET:HE2	1:A:125:VAL:H	1.84	0.42
1:B:133:LEU:HD21	1:B:233:ARG:NH1	2.35	0.42
1:C:106:SER:HB3	1:C:107:THR:H	1.57	0.42
1:B:432:THR:O	1:B:485:TYR:HA	2.20	0.42
1:B:709:VAL:HG22	1:B:1044:VAL:HG22	2.00	0.42
1:C:654:GLY:O	1:C:657:ILE:HG12	2.19	0.42
1:A:37:SER:OG	1:A:38:HIS:N	2.51	0.42
1:A:61:LEU:HD22	1:A:89:TYR:CD2	2.55	0.42
1:A:939:ALA:O	1:A:943:ASN:N	2.49	0.42
1:B:534:THR:HG23	1:C:961:ASN:HB3	2.01	0.42
1:C:26:ARG:HD2	1:C:77:PHE:HD1	1.83	0.42
1:C:187:VAL:CG2	1:C:217:LEU:HD12	2.50	0.42
1:C:797:LYS:HD2	1:C:797:LYS:HA	1.93	0.42
1:C:849:THR:HG23	1:C:852:MET:HB2	2.01	0.42
1:A:140:VAL:HB	1:A:149:ILE:HB	2.01	0.42
1:B:353:TYR:CE1	1:B:357:TYR:HB2	2.54	0.42
1:B:857:THR:HG21	1:B:1037:GLN:HA	2.02	0.42
3:Q:1:NAG:H61	3:Q:2:NAG:N2	2.35	0.42
1:C:50:SER:O	1:C:52:VAL:HG13	2.20	0.42
1:C:59:HIS:ND1	1:C:86:ASP:OD1	2.51	0.42
1:C:287:LEU:HD11	1:C:301:TYR:CB	2.50	0.42
1:C:915:SER:O	1:C:918:GLN:HG2	2.19	0.42
1:A:41:VAL:HG21	1:A:214:PHE:HE1	1.84	0.42
1:A:900:TYR:CE1	1:C:1062:PRO:HB3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:84:PHE:CD2	1:C:88:ILE:HG23	2.55	0.42
1:C:521:ILE:HB	1:C:526:VAL:HG11	2.01	0.42
1:A:856:TYR:CE2	1:C:682:LEU:HD22	2.55	0.42
1:A:1074:ARG:HG2	1:A:1102:ASN:O	2.20	0.42
1:B:960:LEU:HA	1:B:963:ILE:HD12	2.01	0.42
1:B:223:LEU:HA	1:B:224:PRO:HD3	1.85	0.41
1:B:319:ASN:N	1:B:567:LYS:HZ1	2.18	0.41
1:B:888:ARG:HD3	1:B:1032:LEU:O	2.20	0.41
1:B:940:GLN:HE21	1:B:940:GLN:HB3	1.64	0.41
1:C:43:TYR:CE1	1:C:216:ALA:HB1	2.55	0.41
1:A:73:PHE:HA	1:A:249:SER:O	2.20	0.41
1:B:306:PHE:HD2	1:B:602:VAL:HG21	1.85	0.41
1:B:956:ILE:HG12	1:B:975:GLN:HG3	2.02	0.41
1:C:162:PHE:CE2	1:C:224:PRO:HD2	2.54	0.41
1:A:141:VAL:O	1:A:239:PHE:HA	2.21	0.41
1:A:720:ASP:OD2	1:A:722:ASN:N	2.53	0.41
1:B:412:LYS:O	1:B:451:PRO:HA	2.19	0.41
1:B:653:ILE:HB	1:B:657:ILE:O	2.20	0.41
1:B:961:ASN:HA	1:B:964:LEU:HG	2.03	0.41
1:A:131:PHE:HA	1:A:158:PHE:HD2	1.86	0.41
1:A:516:LEU:HD12	1:A:516:LEU:HA	1.89	0.41
1:C:528:PHE:HB2	1:C:530:PHE:CE1	2.56	0.41
1:A:39:ARG:O	1:A:61:LEU:HD23	2.20	0.41
1:A:43:TYR:O	1:A:198:TYR:HE2	2.03	0.41
1:A:603:ASN:HD22	4:A:1302:NAG:C7	2.34	0.41
1:A:694:THR:O	1:B:880:PRO:HD3	2.21	0.41
1:B:194:PHE:CD2	1:B:222:LYS:HG2	2.54	0.41
1:B:1021:LYS:O	1:B:1022:ARG:C	2.59	0.41
1:A:181:LYS:HE3	1:A:203:PRO:O	2.21	0.41
1:B:531:ASN:OD1	1:B:566:PRO:HG3	2.20	0.41
1:C:117:ILE:HG23	1:C:126:ILE:HG22	2.02	0.41
1:C:957:SER:OG	1:C:958:SER:N	2.54	0.41
1:A:59:HIS:HE1	1:A:258:LEU:O	2.03	0.41
1:A:264:MET:HE2	1:A:264:MET:HB3	1.78	0.41
1:A:877:LEU:HD11	1:C:698:PRO:HG3	2.03	0.41
1:A:1125:GLN:H	1:A:1125:GLN:HG2	1.71	0.41
1:B:519:ASP:OD2	1:B:519:ASP:N	2.53	0.41
1:B:700:ASN:OD1	1:B:701:PHE:N	2.49	0.41
1:C:554:ARG:HD3	1:C:558:ASP:OD1	2.19	0.41
1:C:775:PRO:HD3	1:C:862:SER:HB2	2.02	0.41
1:C:867:ALA:HA	1:C:878:GLN:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1115:ILE:HD12	1:C:1115:ILE:HA	1.87	0.41
1:A:967:LEU:HD23	1:A:967:LEU:HA	1.85	0.41
1:B:708:GLU:OE2	1:B:1011:LYS:HE2	2.21	0.41
1:A:139:PHE:O	1:A:237:THR:HA	2.20	0.40
1:A:139:PHE:N	1:A:236:LEU:O	2.49	0.40
1:A:214:PHE:HZ	1:A:273:ILE:HG22	1.86	0.40
1:A:788:ILE:H	1:A:788:ILE:HG12	1.76	0.40
1:C:73:PHE:HD2	1:C:75:LEU:HG	1.86	0.40
1:C:238:ALA:C	1:C:240:PRO:HD3	2.42	0.40
1:C:307:ARG:HA	1:C:307:ARG:HD2	1.91	0.40
1:C:670:THR:HG22	1:C:670:THR:O	2.21	0.40
1:A:976:ILE:HG22	1:A:980:ILE:HD11	2.02	0.40
1:A:1126:PRO:HB2	1:A:1127:GLU:OE1	2.21	0.40
1:B:449:LEU:HD23	1:B:449:LEU:HA	1.87	0.40
1:C:125:VAL:HG21	4:C:1309:NAG:H62	2.04	0.40
1:C:190:ASN:HA	1:C:195:LEU:HD23	2.02	0.40
1:C:275:ASP:OD1	1:C:276:ALA:N	2.54	0.40
1:C:949:LEU:HD23	1:C:949:LEU:HA	1.87	0.40
1:A:118:MET:HB3	1:A:139:PHE:CZ	2.54	0.40
1:A:719:VAL:HA	1:A:840:GLY:O	2.21	0.40
1:A:976:ILE:HG22	1:A:980:ILE:CD1	2.51	0.40
1:B:367:CYS:HA	1:B:420:CYS:HA	2.04	0.40
1:B:567:LYS:HD2	1:B:567:LYS:N	2.36	0.40
1:B:769:LYS:HG3	1:B:770:GLN:HG2	2.04	0.40
1:C:539:LEU:HD23	1:C:539:LEU:HA	1.97	0.40
1:A:62:PRO:CD	1:A:259:LYS:HG3	2.51	0.40
1:A:182:ASP:OD1	1:A:201:TYR:OH	2.39	0.40
1:A:989:THR:HG22	1:B:988:GLN:NE2	2.37	0.40
1:C:100:ARG:HG2	1:C:237:THR:HG23	2.03	0.40
1:B:279:CYS:HA	1:B:285:ALA:HB1	2.03	0.40
1:B:787:GLN:H	1:B:787:GLN:HG2	1.72	0.40
1:B:1011:LYS:HE3	1:B:1025:PHE:O	2.21	0.40
1:C:59:HIS:HA	1:C:260:PRO:HA	2.03	0.40
1:C:307:ARG:NH1	1:C:579:PHE:HB3	2.34	0.40

There are no symmetry-related clashes.



## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	860/1271 (68%)	807 (94%)	52 (6%)	1 (0%)	48	81
1	B	1061/1271 (84%)	1022 (96%)	37 (4%)	2 (0%)	44	76
1	C	863/1271 (68%)	826 (96%)	37 (4%)	0	100	100
All	All	2784/3813 (73%)	2655 (95%)	126 (4%)	3 (0%)	50	81

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	604	CYS
1	B	246	TRP
1	B	722	ASN

### 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	759/1100 (69%)	741 (98%)	18 (2%)	44	62
1	B	931/1100 (85%)	908 (98%)	23 (2%)	42	61
1	C	760/1100 (69%)	737 (97%)	23 (3%)	36	57
All	All	2450/3300 (74%)	2386 (97%)	64 (3%)	42	61

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	LEU
1	A	33	GLN
1	A	54	HIS
1	A	60	PHE
1	A	102	TRP
1	A	118	MET
1	A	297	ASP
1	A	317	PHE
1	A	558	ASP
1	A	607	VAL
1	A	627	ASN
1	A	668	ARG
1	A	748	ARG
1	A	756	GLU
1	A	887	TYR
1	A	933	ASP
1	A	958	SER
1	A	1101	ASP
1	B	118	MET
1	B	158	PHE
1	B	194	PHE
1	B	232	PHE
1	B	233	ARG
1	B	353	TYR
1	B	366	LYS
1	B	380	PHE
1	B	477	TRP
1	B	481	ASP
1	B	525	CYS
1	B	604	CYS
1	B	662	HIS
1	B	665	SER
1	B	723	MET
1	B	759	ARG
1	B	839	ASN
1	B	890	ASN
1	B	935	VAL
1	B	948	GLN
1	B	994	GLN
1	B	1026	CYS
1	B	1067	GLU
1	C	33	GLN
1	C	106	SER

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Mol	Chain	Res	Type
1	C	108	MET
1	C	167	LYS
1	C	221	PHE
1	C	232	PHE
1	C	294	PHE
1	C	304	SER
1	C	519	ASP
1	C	540	THR
1	C	558	ASP
1	C	650	ASP
1	C	668	ARG
1	C	731	GLU
1	C	756	GLU
1	C	773	LYS
1	C	786	SER
1	C	837	LYS
1	C	838	PHE
1	C	948	GLN
1	C	958	SER
1	C	960	LEU
1	C	987	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	159	ASN
1	A	994	GLN
1	B	76	ASN
1	B	397	GLN
1	B	938	ASN
1	B	940	GLN
1	B	994	GLN
1	C	54	HIS
1	C	722	ASN
1	C	745	GLN
1	C	747	ASN
1	C	988	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 ⓘ

35 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	2,1	14,14,15	0.25	0	17,19,21	0.39	0
2	NAG	D	2	2	14,14,15	0.23	0	17,19,21	0.42	0
2	NAG	E	1	2,1	14,14,15	0.44	0	17,19,21	0.57	0
2	NAG	E	2	2	14,14,15	0.22	0	17,19,21	0.42	0
2	NAG	F	1	2,1	14,14,15	0.18	0	17,19,21	0.47	0
2	NAG	F	2	2	14,14,15	0.51	0	17,19,21	1.25	1 (5%)
2	NAG	G	1	2,1	14,14,15	0.36	0	17,19,21	0.50	0
2	NAG	G	2	2	14,14,15	0.22	0	17,19,21	0.38	0
2	NAG	H	1	2,1	14,14,15	0.60	0	17,19,21	0.81	1 (5%)
2	NAG	H	2	2	14,14,15	0.28	0	17,19,21	0.41	0
2	NAG	I	1	2,1	14,14,15	0.79	1 (7%)	17,19,21	0.83	1 (5%)
2	NAG	I	2	2	14,14,15	0.25	0	17,19,21	0.53	0
2	NAG	J	1	2,1	14,14,15	0.22	0	17,19,21	0.69	0
2	NAG	J	2	2	14,14,15	0.31	0	17,19,21	0.60	1 (5%)
3	NAG	K	1	3,1	14,14,15	0.21	0	17,19,21	0.42	0
3	NAG	K	2	3	14,14,15	0.25	0	17,19,21	0.51	0
3	BMA	K	3	3	11,11,12	0.64	0	15,15,17	0.73	0
3	NAG	L	1	3,1	14,14,15	0.24	0	17,19,21	0.44	0
3	NAG	L	2	3	14,14,15	0.20	0	17,19,21	0.49	0
3	BMA	L	3	3	11,11,12	0.66	0	15,15,17	0.71	0
2	NAG	M	1	2,1	14,14,15	0.30	0	17,19,21	0.58	0
2	NAG	M	2	2	14,14,15	0.25	0	17,19,21	0.42	0
2	NAG	N	1	2,1	14,14,15	0.26	0	17,19,21	0.44	0
2	NAG	N	2	2	14,14,15	0.17	0	17,19,21	0.47	0
2	NAG	O	1	2,1	14,14,15	0.47	0	17,19,21	0.44	0
2	NAG	O	2	2	14,14,15	0.28	0	17,19,21	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	P	1	2,1	14,14,15	0.35	0	17,19,21	0.44	0
2	NAG	P	2	2	14,14,15	0.24	0	17,19,21	0.40	0
3	NAG	Q	1	3,1	14,14,15	0.26	0	17,19,21	0.59	0
3	NAG	Q	2	3	14,14,15	0.18	0	17,19,21	0.42	0
3	BMA	Q	3	3	11,11,12	0.63	0	15,15,17	0.65	0
2	NAG	R	1	2,1	14,14,15	0.26	0	17,19,21	0.49	0
2	NAG	R	2	2	14,14,15	0.32	0	17,19,21	0.44	0
2	NAG	S	1	2,1	14,14,15	0.24	0	17,19,21	0.38	0
2	NAG	S	2	2	14,14,15	0.20	0	17,19,21	0.42	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	2,1	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	NAG	E	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	NAG	F	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	F	2	2	-	5/6/23/26	0/1/1/1
2	NAG	G	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	2/6/23/26	0/1/1/1
2	NAG	H	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	H	2	2	-	2/6/23/26	0/1/1/1
2	NAG	I	1	2,1	-	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	2,1	-	0/6/23/26	0/1/1/1
2	NAG	J	2	2	-	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	-	2/6/23/26	0/1/1/1
3	BMA	K	3	3	-	0/2/19/22	0/1/1/1
3	NAG	L	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	L	2	3	-	0/6/23/26	0/1/1/1
3	BMA	L	3	3	-	0/2/19/22	0/1/1/1
2	NAG	M	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	M	2	2	-	0/6/23/26	0/1/1/1
2	NAG	N	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	N	2	2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	O	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	O	2	2	-	0/6/23/26	0/1/1/1
2	NAG	P	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	P	2	2	-	0/6/23/26	0/1/1/1
3	NAG	Q	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	2/6/23/26	0/1/1/1
3	BMA	Q	3	3	-	0/2/19/22	0/1/1/1
2	NAG	R	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	R	2	2	-	0/6/23/26	0/1/1/1
2	NAG	S	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	S	2	2	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	1	NAG	O5-C1	-2.65	1.39	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	2	NAG	C2-N2-C7	4.23	128.93	122.90
2	H	1	NAG	C1-O5-C5	2.38	115.41	112.19
2	I	1	NAG	C3-C4-C5	2.23	114.22	110.24
2	J	2	NAG	C1-O5-C5	2.10	115.04	112.19

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	2	NAG	O5-C5-C6-O6
2	I	2	NAG	O5-C5-C6-O6
2	G	2	NAG	O5-C5-C6-O6
2	J	2	NAG	O5-C5-C6-O6
3	Q	2	NAG	O5-C5-C6-O6
2	P	1	NAG	C4-C5-C6-O6
2	P	1	NAG	O5-C5-C6-O6
2	H	2	NAG	C4-C5-C6-O6
2	F	2	NAG	O5-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	O	1	NAG	O5-C5-C6-O6

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

There are no ring outliers.

9 monomers are involved in 7 short contacts:

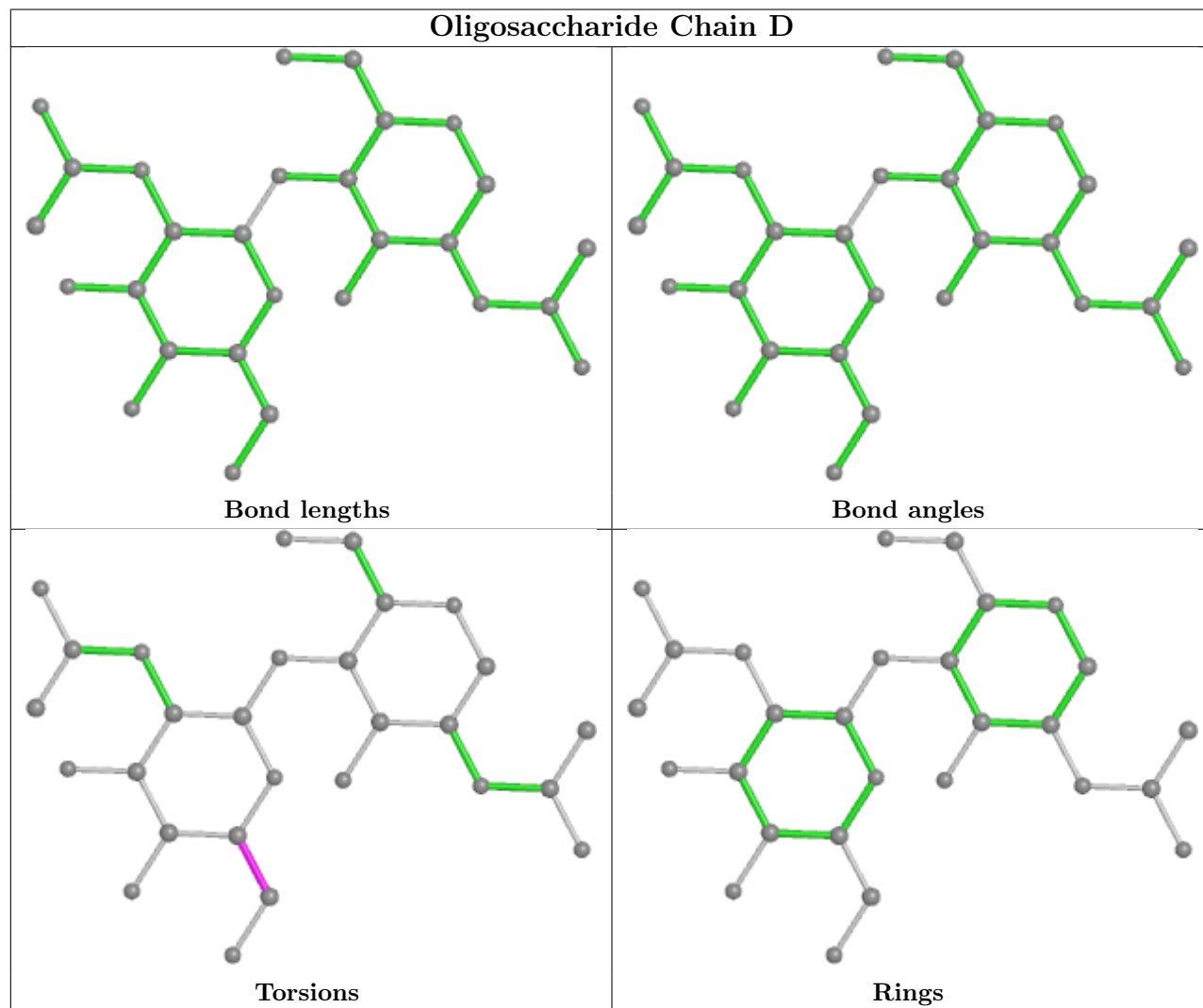
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	O	1	NAG	1	0
2	R	1	NAG	1	0
2	N	1	NAG	1	0
3	Q	1	NAG	1	0
2	I	2	NAG	1	0
2	E	1	NAG	1	0
2	F	2	NAG	1	0

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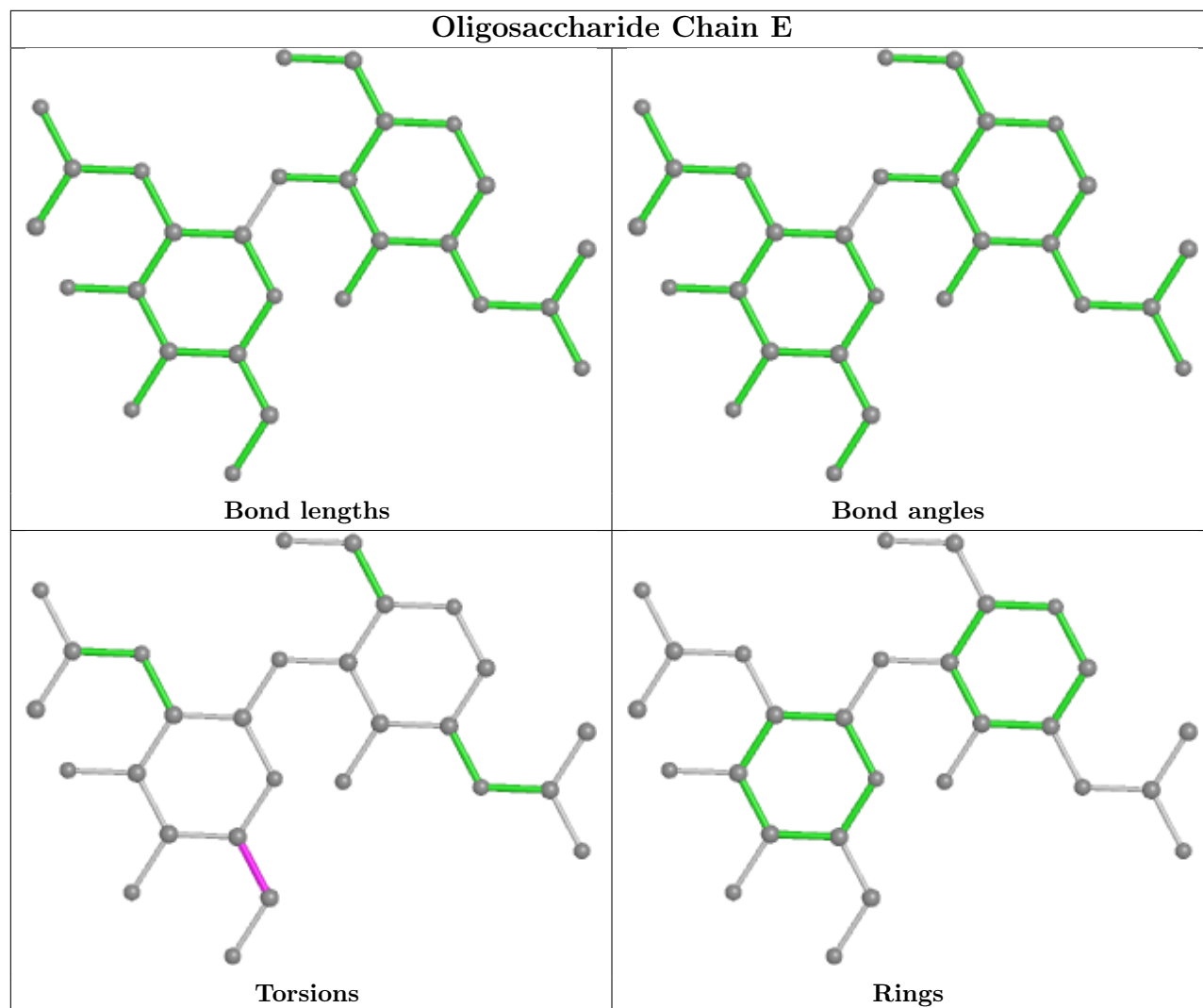
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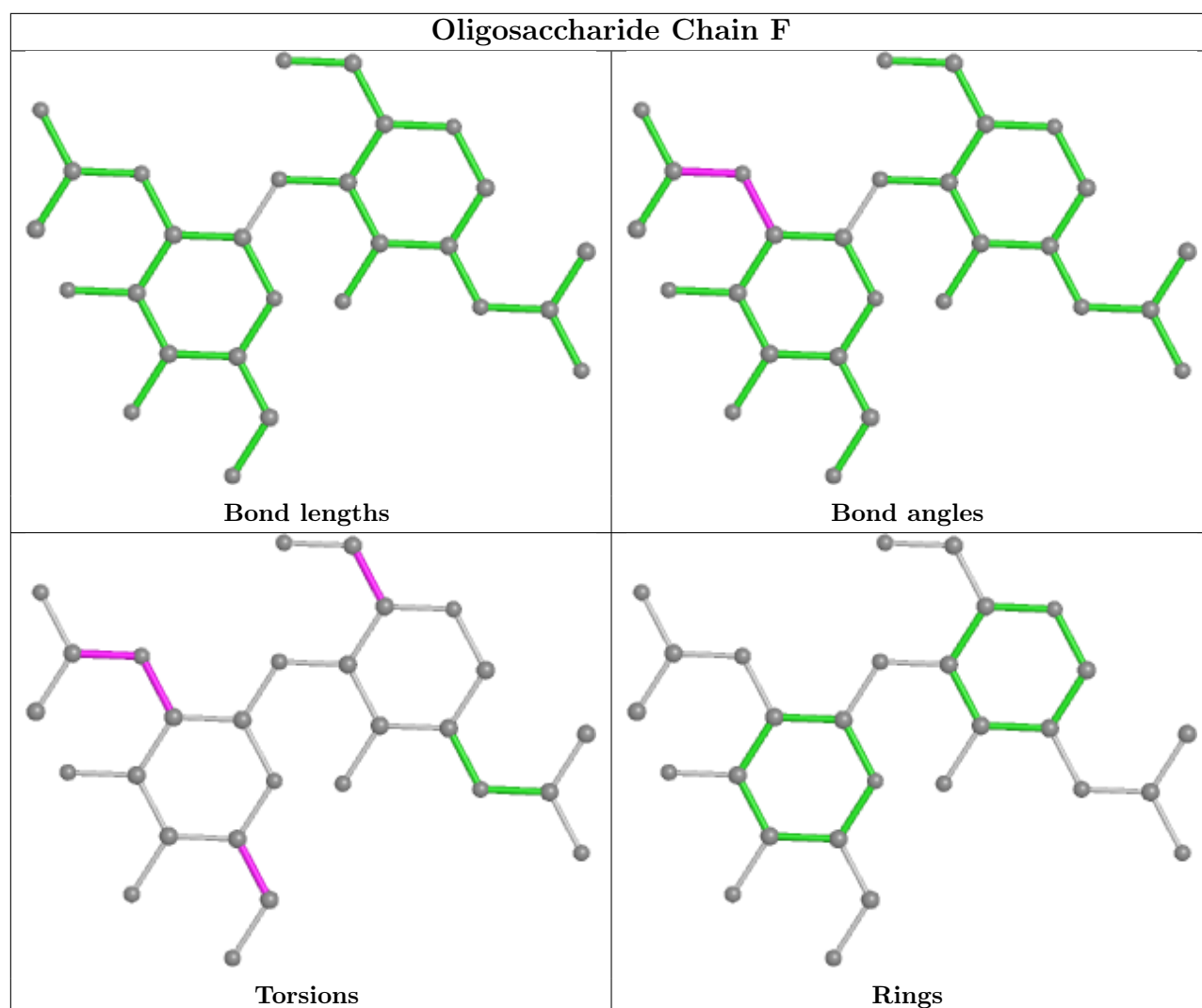
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	Q	2	NAG	1	0
2	I	1	NAG	1	0

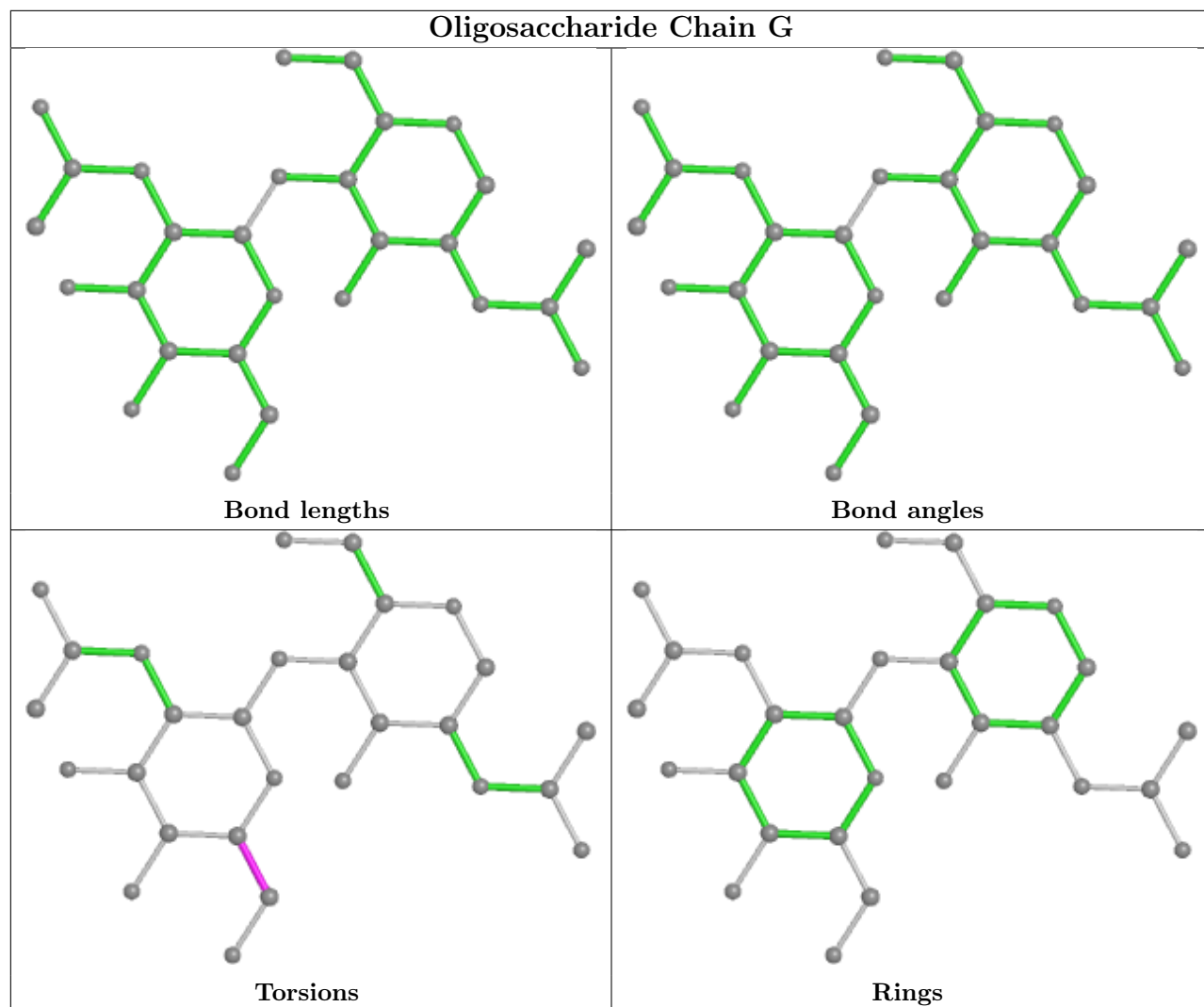
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

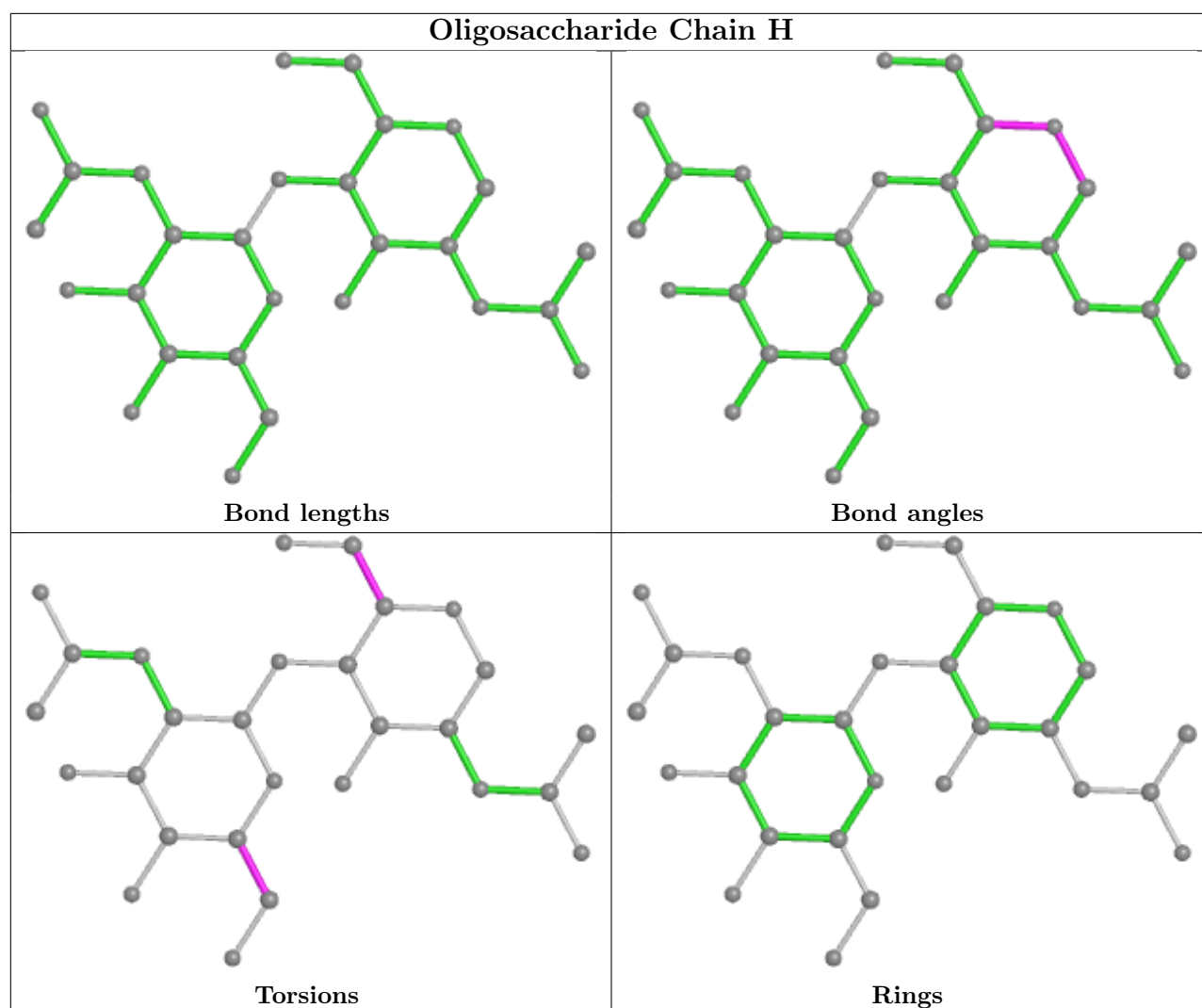


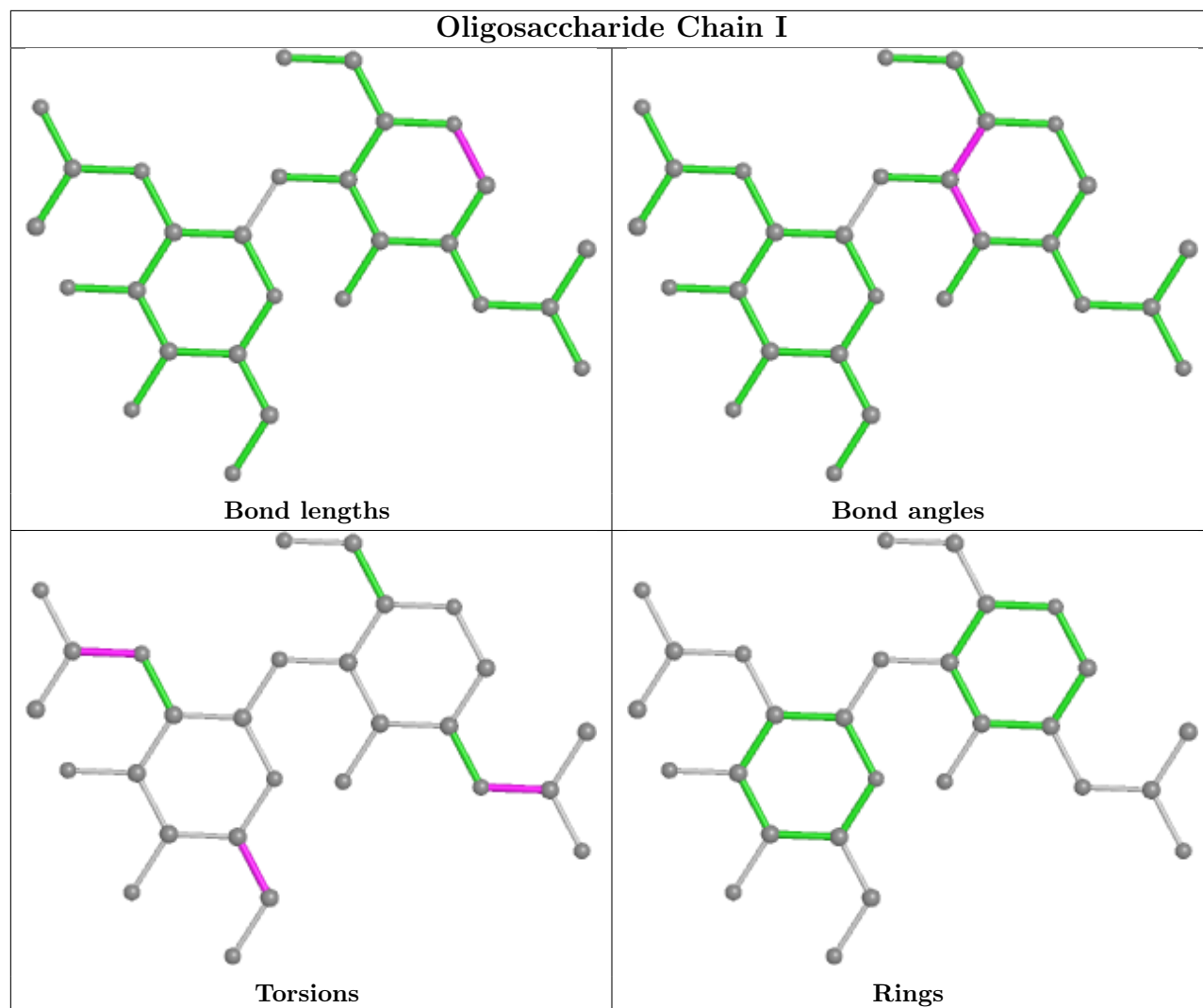


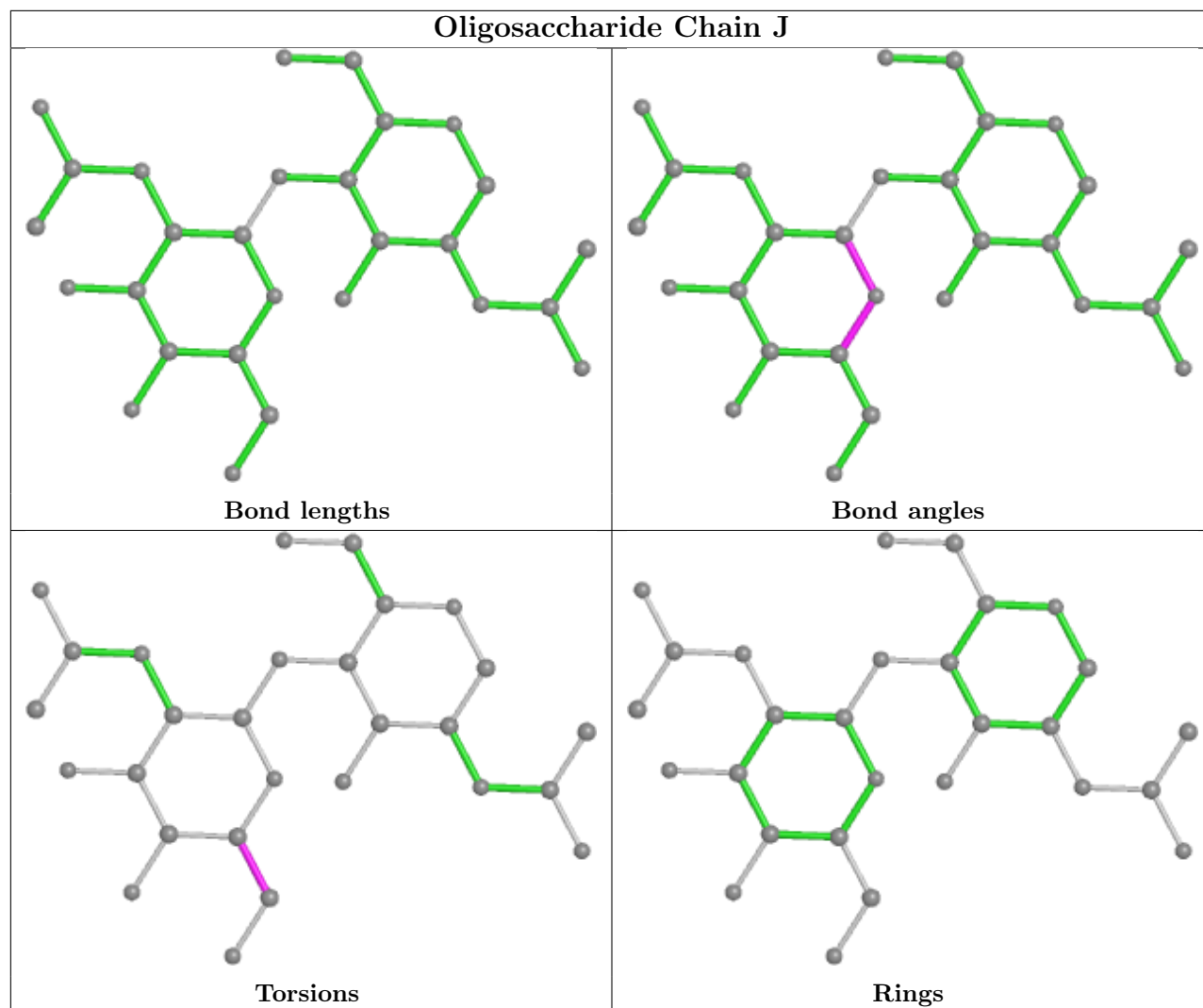


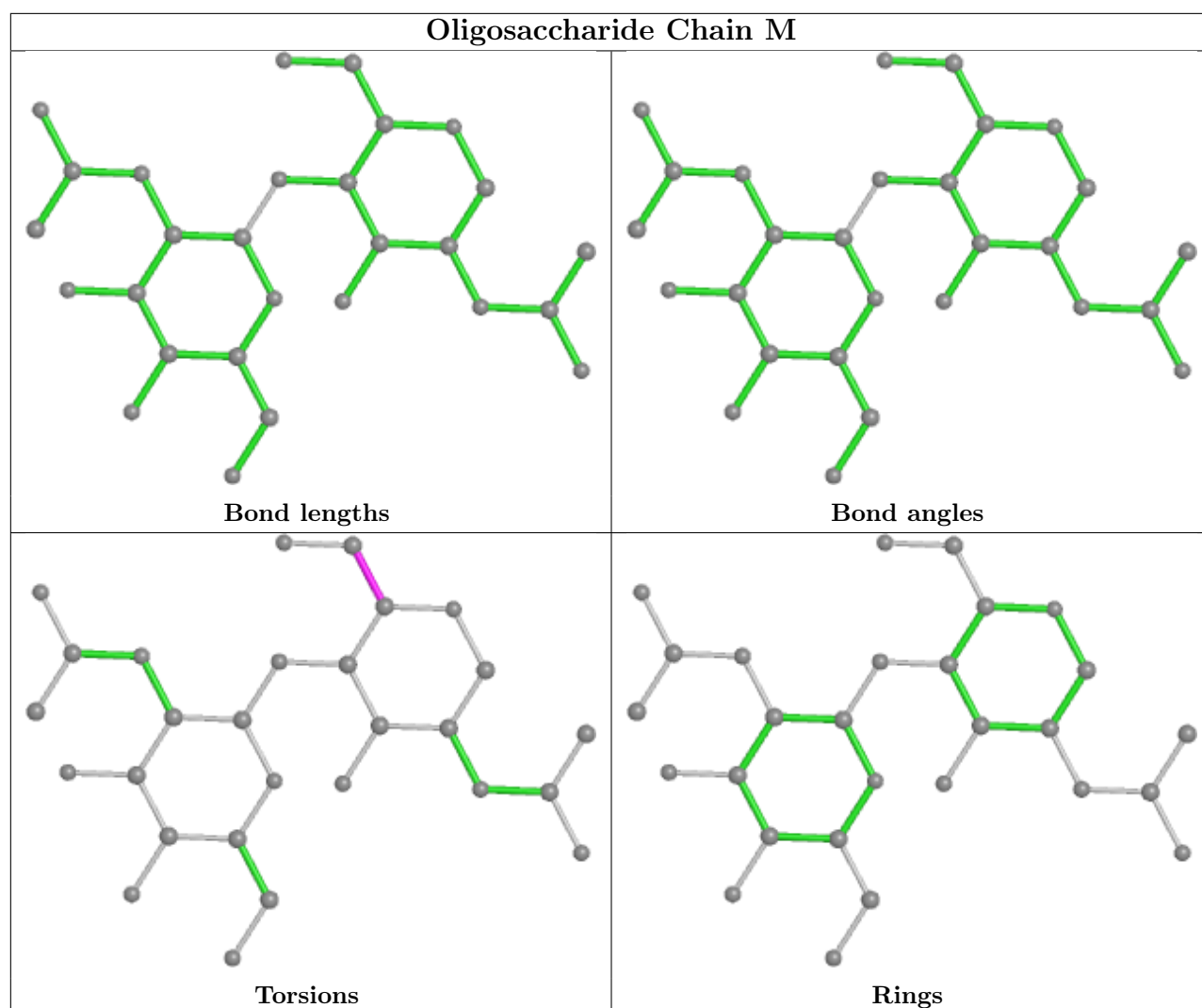


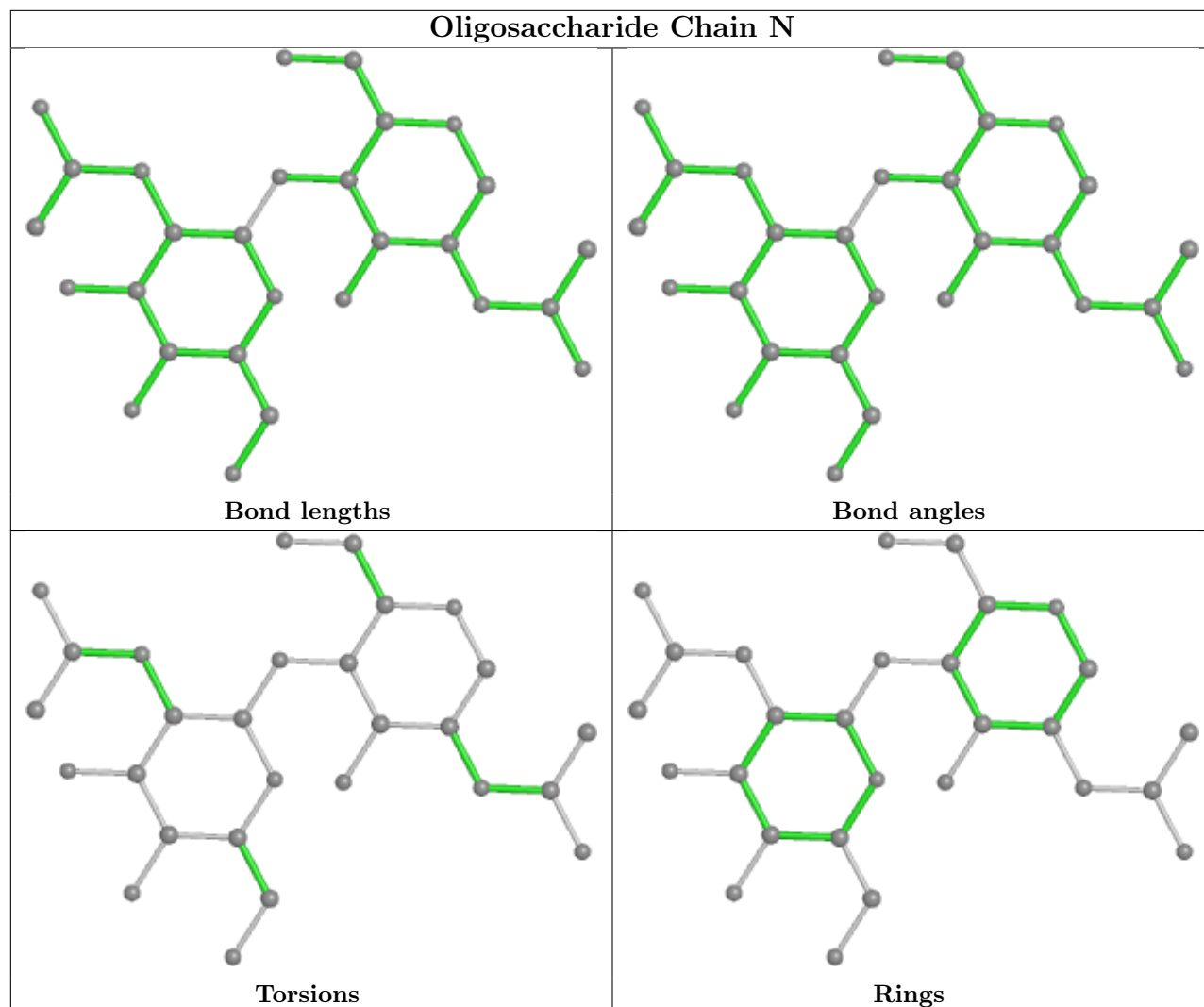




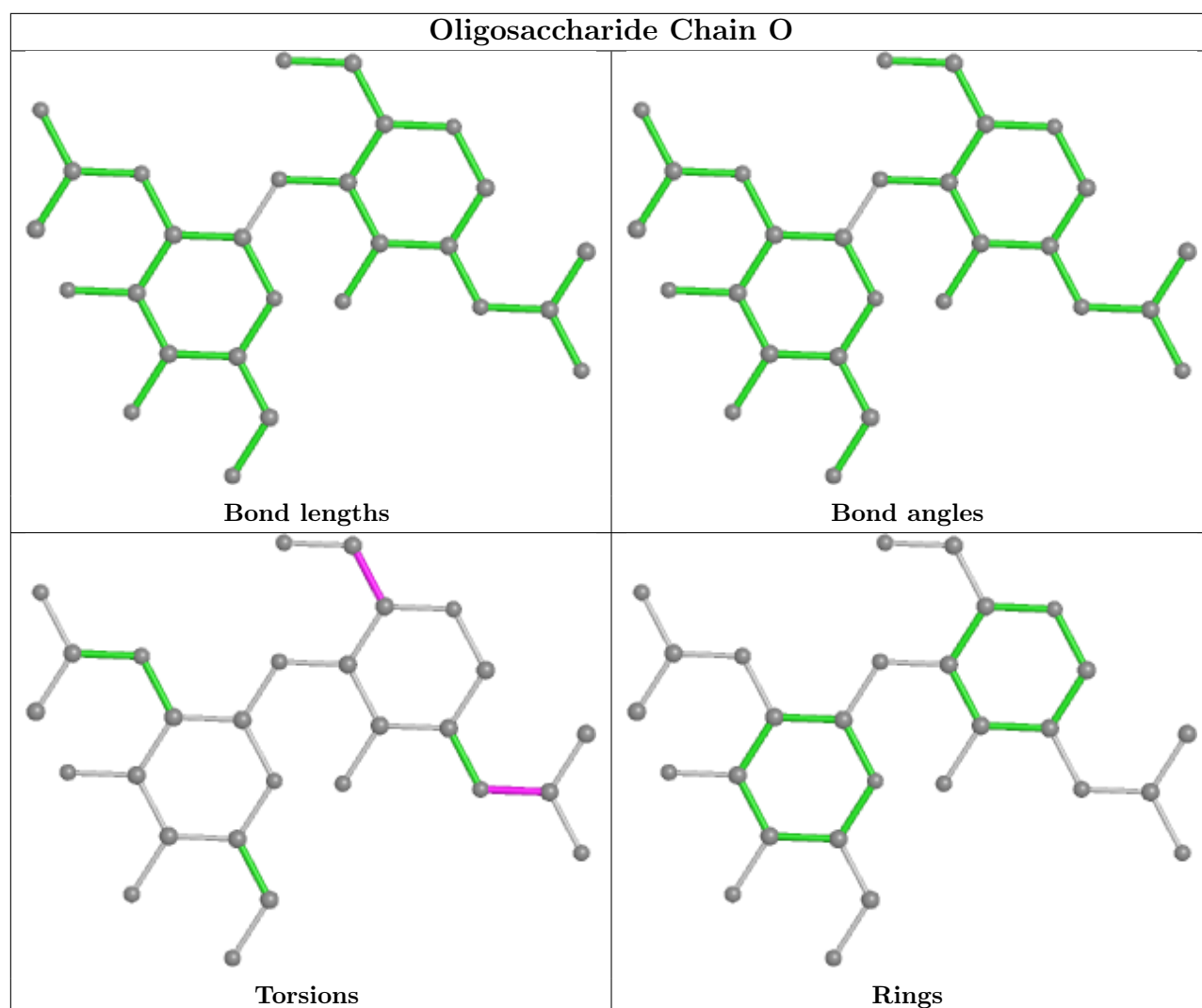


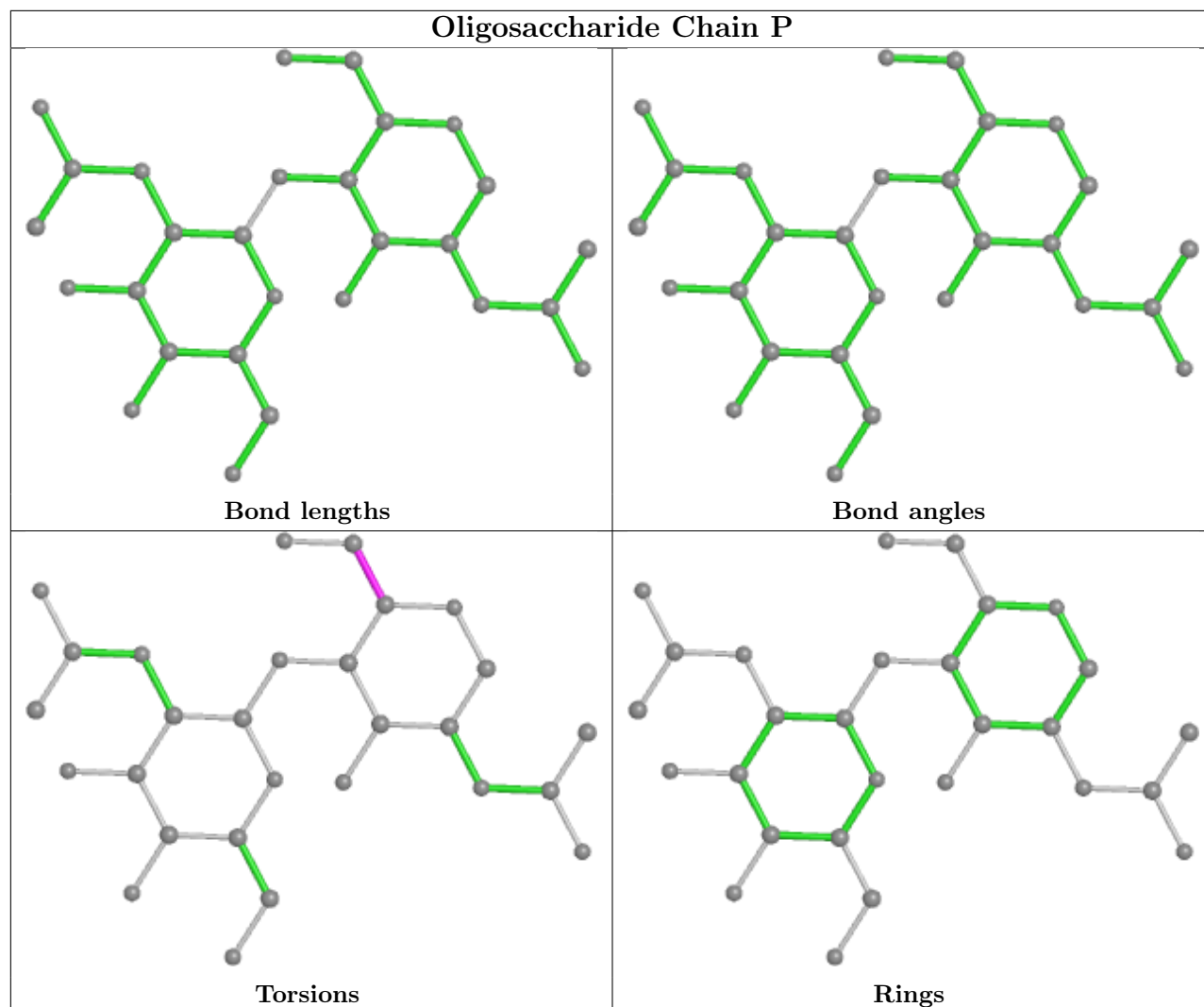


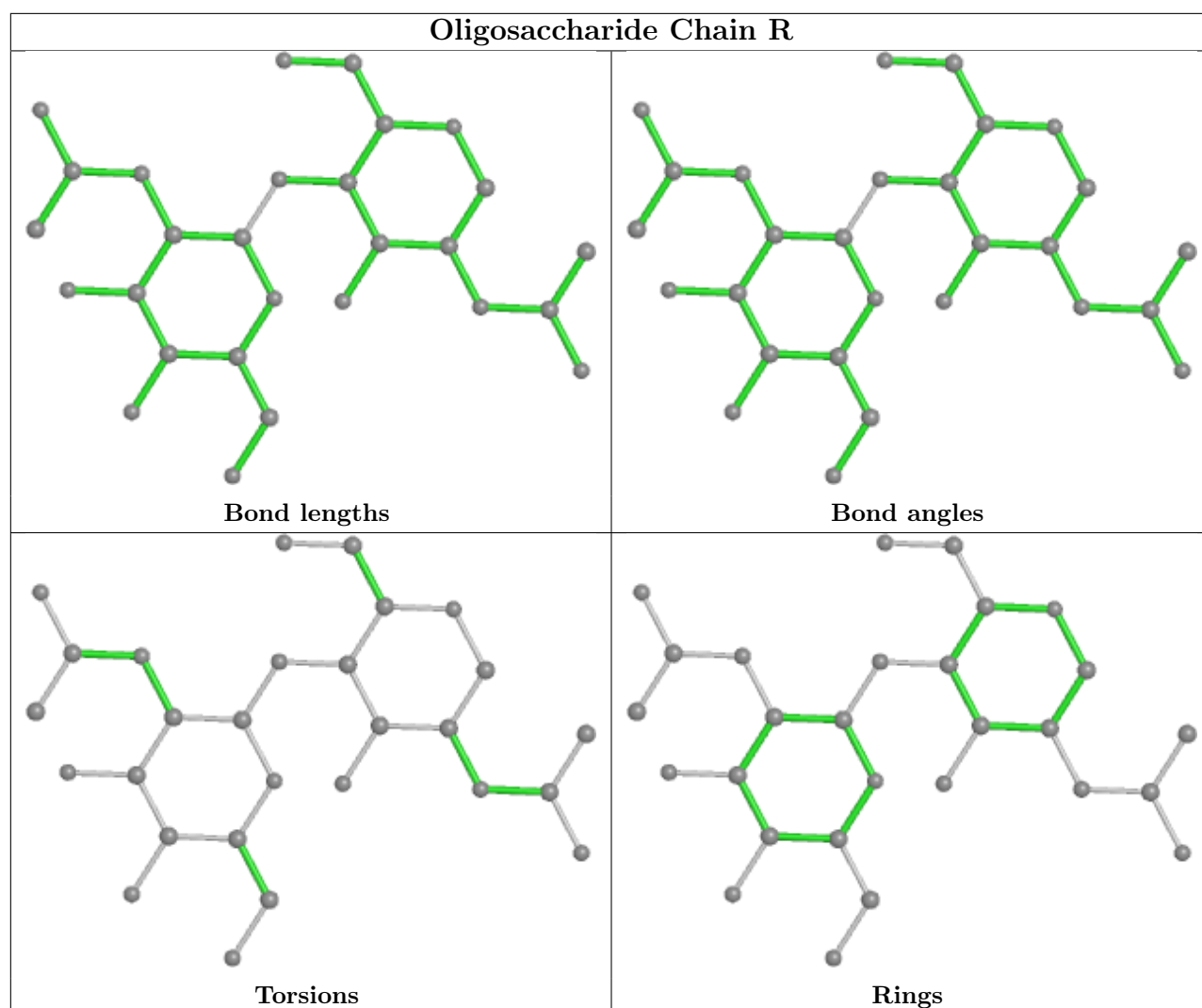


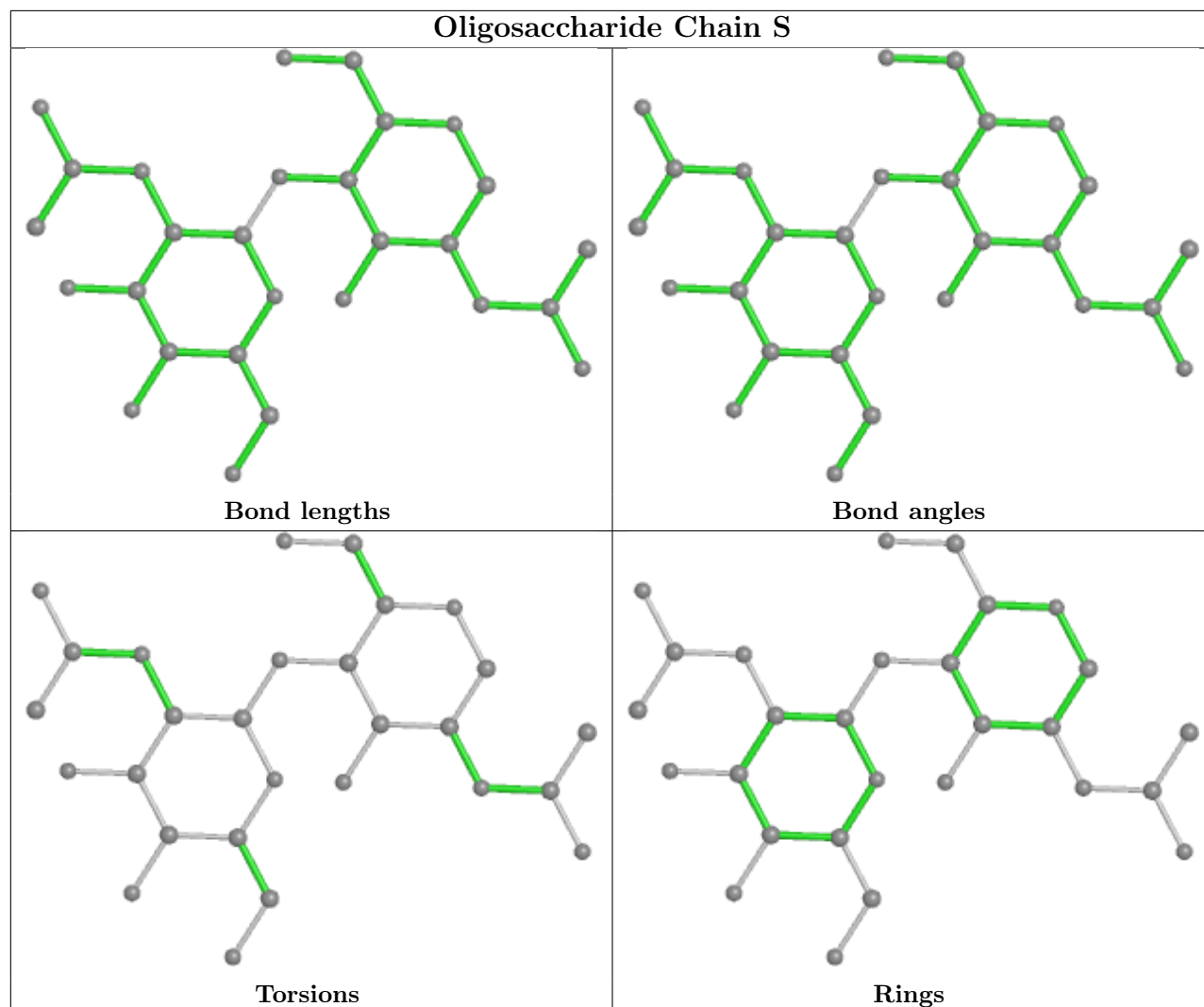


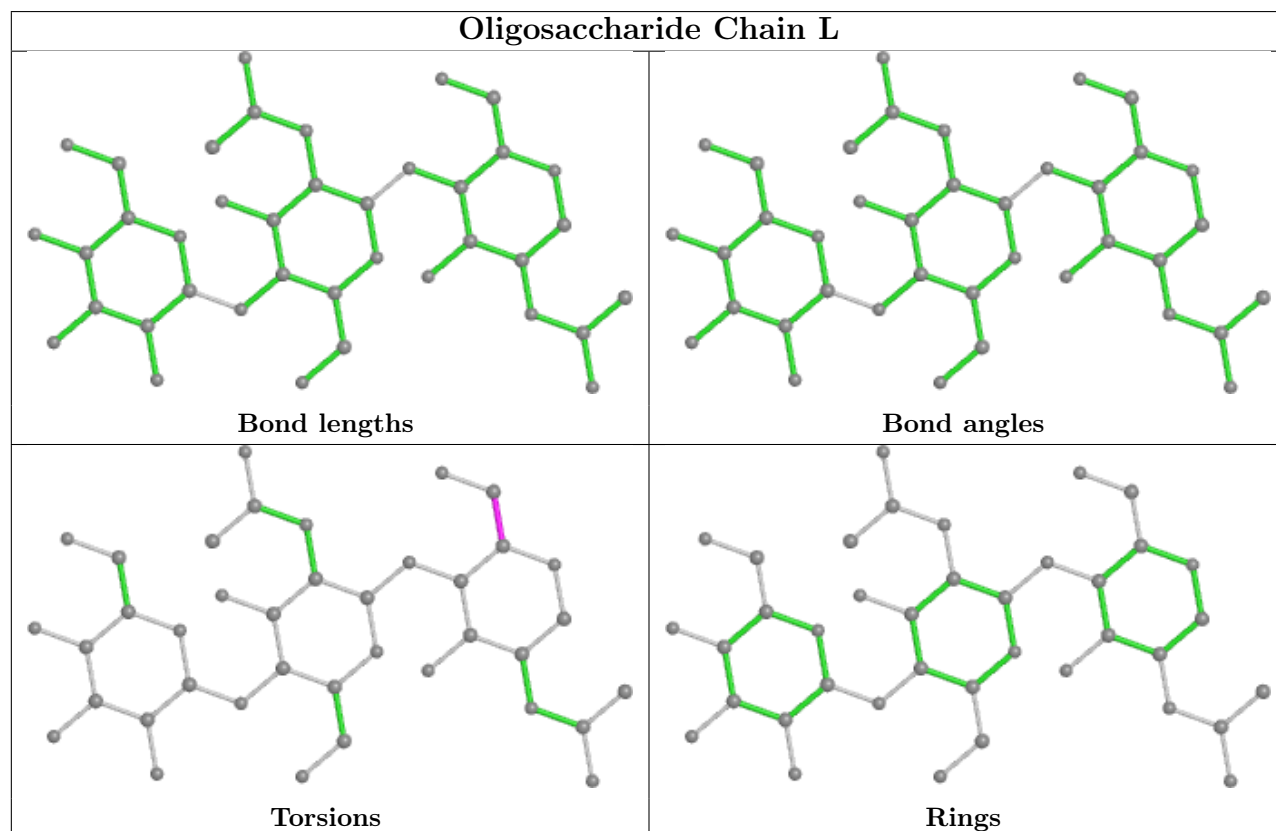
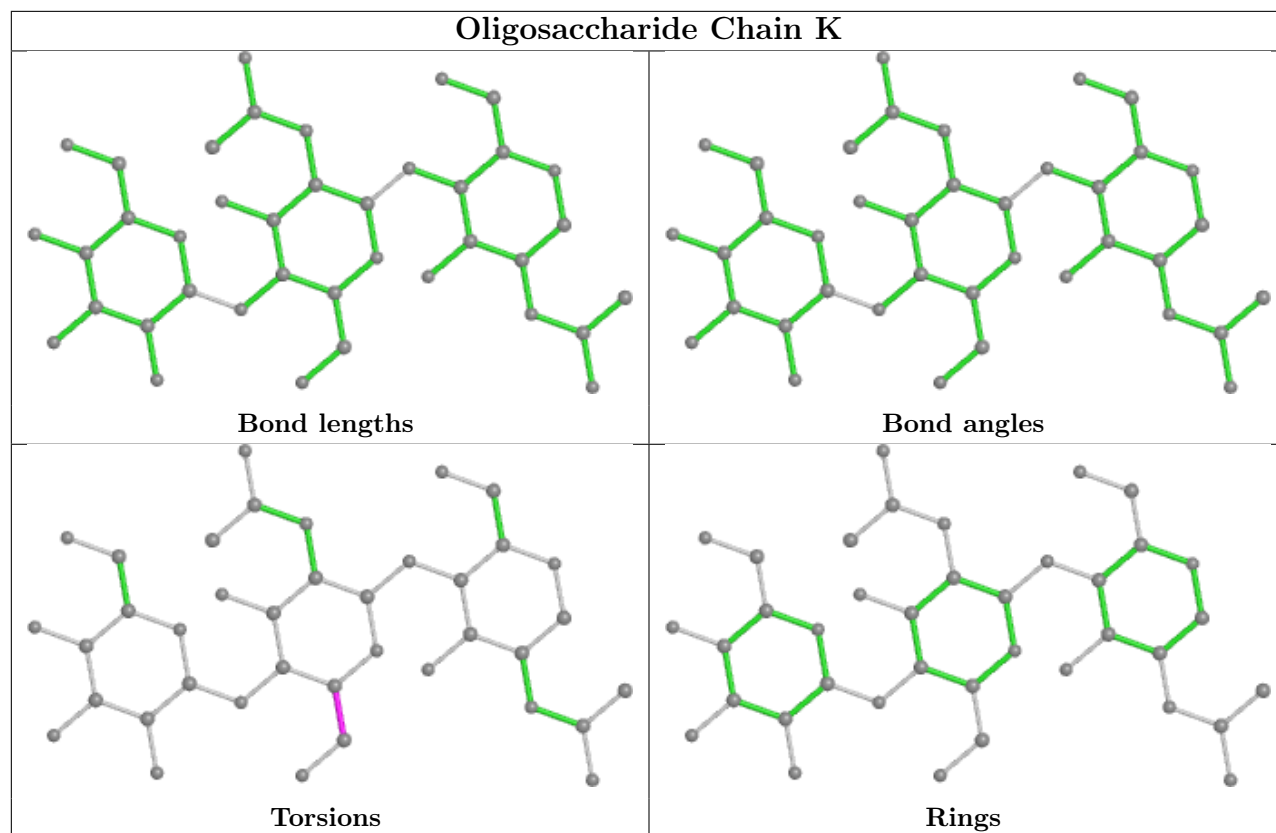


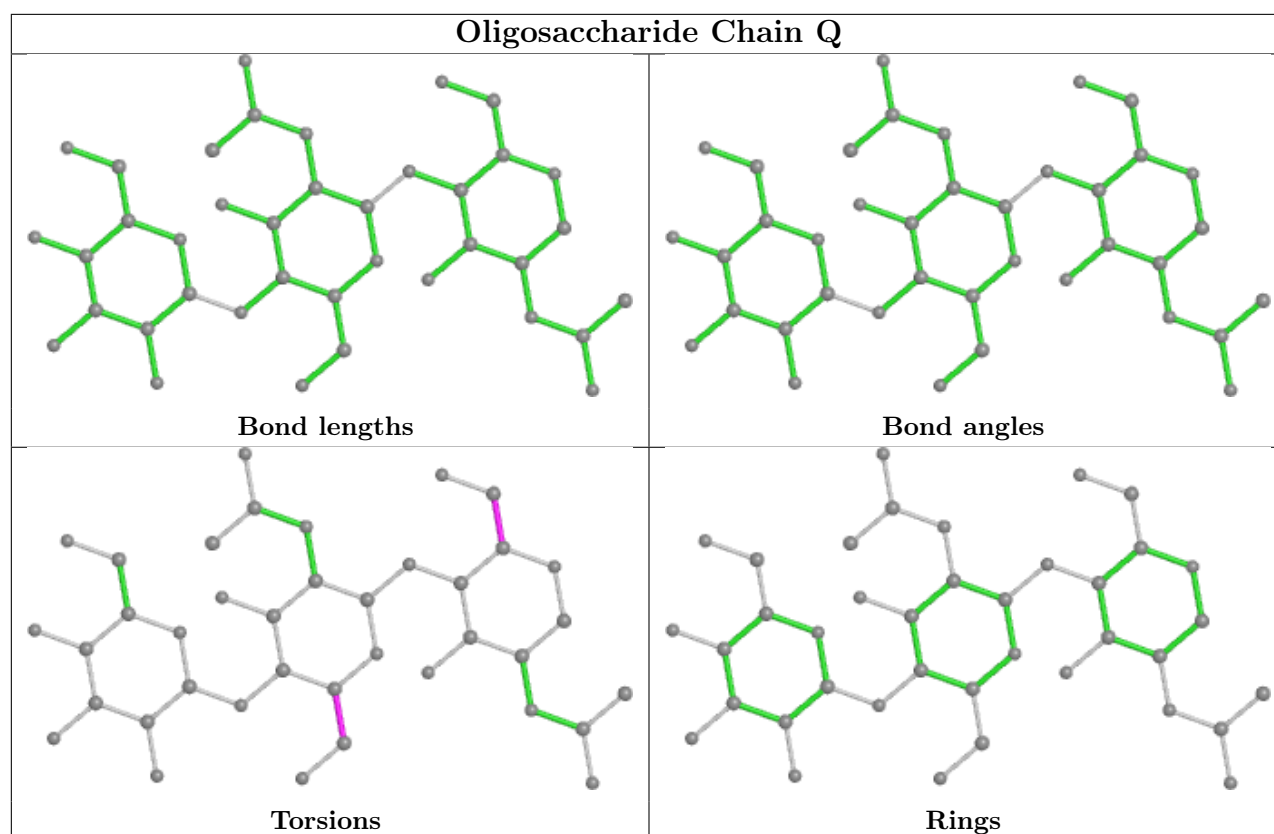












## 5.6 Ligand geometry [i](#)

19 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	0.18	0	17,19,21	0.55	0
4	NAG	C	1301	1	14,14,15	0.27	0	17,19,21	0.41	0
4	NAG	C	1309	1	14,14,15	0.17	0	17,19,21	0.41	0
4	NAG	C	1306	1	14,14,15	0.21	0	17,19,21	0.42	0
4	NAG	C	1302	1	14,14,15	0.32	0	17,19,21	0.33	0
4	NAG	A	1304	1	14,14,15	0.24	0	17,19,21	0.35	0
4	NAG	C	1307	1	14,14,15	0.28	0	17,19,21	0.34	0
4	NAG	C	1308	1	14,14,15	0.33	0	17,19,21	0.43	0
4	NAG	B	1303	1	14,14,15	0.18	0	17,19,21	0.43	0
4	NAG	C	1303	1	14,14,15	0.17	0	17,19,21	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	B	1301	1	14,14,15	0.19	0	17,19,21	0.37	0
4	NAG	C	1305	1	14,14,15	0.17	0	17,19,21	0.43	0
4	NAG	A	1301	1	14,14,15	0.18	0	17,19,21	0.42	0
4	NAG	B	1306	1	14,14,15	0.20	0	17,19,21	0.40	0
4	NAG	B	1302	1	14,14,15	0.17	0	17,19,21	0.47	0
4	NAG	B	1304	1	14,14,15	0.22	0	17,19,21	0.48	0
4	NAG	C	1304	1	14,14,15	0.21	0	17,19,21	0.56	0
4	NAG	A	1303	1	14,14,15	0.22	0	17,19,21	0.41	0
4	NAG	A	1302	1	14,14,15	0.23	0	17,19,21	0.37	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
4	NAG	B	1305	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1301	1	-	4/6/23/26	0/1/1/1
4	NAG	C	1309	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1306	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1302	1	-	4/6/23/26	0/1/1/1
4	NAG	A	1304	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1307	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1308	1	-	4/6/23/26	0/1/1/1
4	NAG	B	1303	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1303	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1301	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1305	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1301	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1306	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1302	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1304	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1304	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1303	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1302	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (33) torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1309	NAG	2	0
4	A	1302	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.