



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 06:05 AM UTC

PDB ID : 7K9H / pdb_00007k9h
EMDB ID : EMD-22748
Title : SARS-CoV-2 Spike in complex with neutralizing Fab 2B04 (one up, two down conformation)
Authors : Errico, J.M.; Fremont, D.H.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : 2020-09-29
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 : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

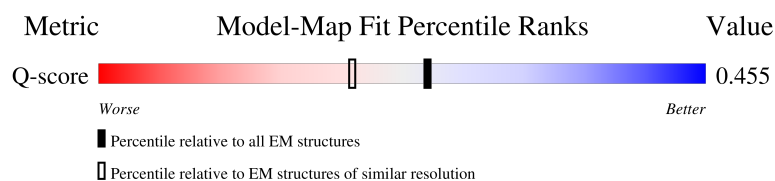
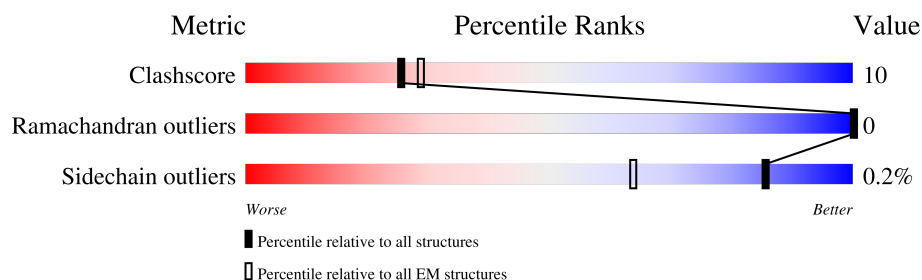
1 Overall quality at a glance

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15020 (2.70 - 3.70)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1256	 63% 12% 24%
1	B	1256	 63% 17% 21%
1	C	1256	 63% 16% 21%
2	H	119	 12% 56% 44%

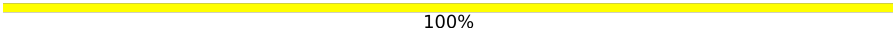
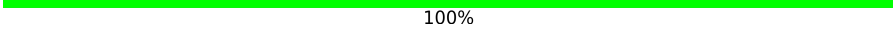
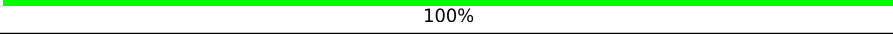
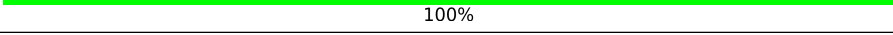
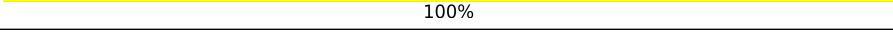
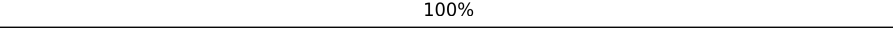
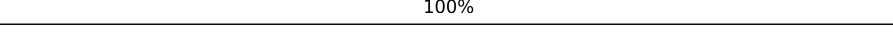
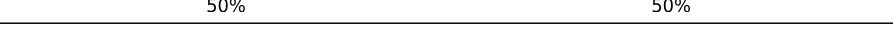
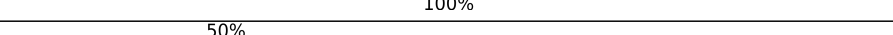
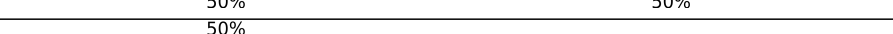
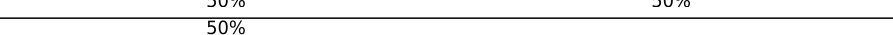
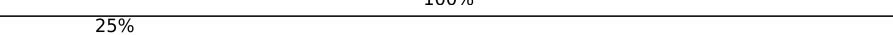
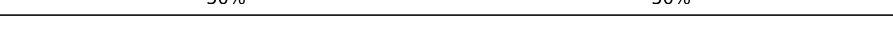
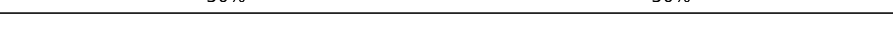
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Mol	Chain	Length	Quality of chain
2	I	119	
3	L	109	
3	M	109	
4	D	3	
4	E	3	
4	S	3	
4	T	3	
4	V	3	
4	W	3	
4	a	3	
4	e	3	
4	h	3	
4	i	3	
4	j	3	
4	m	3	
4	u	3	
4	v	3	
5	F	2	
5	G	2	
5	K	2	
5	N	2	
5	O	2	
5	Q	2	
5	R	2	
5	X	2	

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Mol	Chain	Length	Quality of chain
5	Y	2	
5	Z	2	
5	c	2	
5	d	2	
5	f	2	
5	g	2	
5	k	2	
5	l	2	
5	o	2	
5	p	2	
5	q	2	
5	s	2	
5	t	2	
6	J	2	
6	b	2	
6	n	2	
7	P	4	
7	U	4	
7	r	4	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 27022 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	950	Total	C	N	O	S	0	0
			6876	4373	1165	1306	32		
1	B	994	Total	C	N	O	S	0	0
			7649	4895	1275	1445	34		
1	C	991	Total	C	N	O	S	0	0
			7623	4883	1274	1432	34		

There are 156 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ARG	deletion	UNP P0DTC2
A	?	-	ARG	deletion	UNP P0DTC2
A	?	-	ALA	deletion	UNP P0DTC2
A	685	ALA	ARG	engineered mutation	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
A	1214	SER	-	expression tag	UNP P0DTC2
A	1215	GLY	-	expression tag	UNP P0DTC2
A	1216	ARG	-	expression tag	UNP P0DTC2
A	1217	LEU	-	expression tag	UNP P0DTC2
A	1218	VAL	-	expression tag	UNP P0DTC2
A	1219	PRO	-	expression tag	UNP P0DTC2
A	1220	ARG	-	expression tag	UNP P0DTC2
A	1221	GLY	-	expression tag	UNP P0DTC2
A	1222	SER	-	expression tag	UNP P0DTC2
A	1223	PRO	-	expression tag	UNP P0DTC2
A	1224	GLY	-	expression tag	UNP P0DTC2
A	1225	SER	-	expression tag	UNP P0DTC2
A	1226	GLY	-	expression tag	UNP P0DTC2
A	1227	TYR	-	expression tag	UNP P0DTC2
A	1228	ILE	-	expression tag	UNP P0DTC2
A	1229	PRO	-	expression tag	UNP P0DTC2
A	1230	GLU	-	expression tag	UNP P0DTC2
A	1231	ALA	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1232	PRO	-	expression tag	UNP P0DTC2
A	1233	ARG	-	expression tag	UNP P0DTC2
A	1234	ASP	-	expression tag	UNP P0DTC2
A	1235	GLY	-	expression tag	UNP P0DTC2
A	1236	GLN	-	expression tag	UNP P0DTC2
A	1237	ALA	-	expression tag	UNP P0DTC2
A	1238	TYR	-	expression tag	UNP P0DTC2
A	1239	VAL	-	expression tag	UNP P0DTC2
A	1240	ARG	-	expression tag	UNP P0DTC2
A	1241	LYS	-	expression tag	UNP P0DTC2
A	1242	ASP	-	expression tag	UNP P0DTC2
A	1243	GLY	-	expression tag	UNP P0DTC2
A	1244	GLU	-	expression tag	UNP P0DTC2
A	1245	TRP	-	expression tag	UNP P0DTC2
A	1246	VAL	-	expression tag	UNP P0DTC2
A	1247	LEU	-	expression tag	UNP P0DTC2
A	1248	LEU	-	expression tag	UNP P0DTC2
A	1249	SER	-	expression tag	UNP P0DTC2
A	1250	THR	-	expression tag	UNP P0DTC2
A	1251	PHE	-	expression tag	UNP P0DTC2
A	1252	LEU	-	expression tag	UNP P0DTC2
A	1253	GLY	-	expression tag	UNP P0DTC2
A	1254	HIS	-	expression tag	UNP P0DTC2
A	1255	HIS	-	expression tag	UNP P0DTC2
A	1256	HIS	-	expression tag	UNP P0DTC2
A	1257	HIS	-	expression tag	UNP P0DTC2
A	1258	HIS	-	expression tag	UNP P0DTC2
A	1259	HIS	-	expression tag	UNP P0DTC2
B	?	-	ARG	deletion	UNP P0DTC2
B	?	-	ARG	deletion	UNP P0DTC2
B	?	-	ALA	deletion	UNP P0DTC2
B	685	ALA	ARG	engineered mutation	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	1214	SER	-	expression tag	UNP P0DTC2
B	1215	GLY	-	expression tag	UNP P0DTC2
B	1216	ARG	-	expression tag	UNP P0DTC2
B	1217	LEU	-	expression tag	UNP P0DTC2
B	1218	VAL	-	expression tag	UNP P0DTC2
B	1219	PRO	-	expression tag	UNP P0DTC2
B	1220	ARG	-	expression tag	UNP P0DTC2
B	1221	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1222	SER	-	expression tag	UNP P0DTC2
B	1223	PRO	-	expression tag	UNP P0DTC2
B	1224	GLY	-	expression tag	UNP P0DTC2
B	1225	SER	-	expression tag	UNP P0DTC2
B	1226	GLY	-	expression tag	UNP P0DTC2
B	1227	TYR	-	expression tag	UNP P0DTC2
B	1228	ILE	-	expression tag	UNP P0DTC2
B	1229	PRO	-	expression tag	UNP P0DTC2
B	1230	GLU	-	expression tag	UNP P0DTC2
B	1231	ALA	-	expression tag	UNP P0DTC2
B	1232	PRO	-	expression tag	UNP P0DTC2
B	1233	ARG	-	expression tag	UNP P0DTC2
B	1234	ASP	-	expression tag	UNP P0DTC2
B	1235	GLY	-	expression tag	UNP P0DTC2
B	1236	GLN	-	expression tag	UNP P0DTC2
B	1237	ALA	-	expression tag	UNP P0DTC2
B	1238	TYR	-	expression tag	UNP P0DTC2
B	1239	VAL	-	expression tag	UNP P0DTC2
B	1240	ARG	-	expression tag	UNP P0DTC2
B	1241	LYS	-	expression tag	UNP P0DTC2
B	1242	ASP	-	expression tag	UNP P0DTC2
B	1243	GLY	-	expression tag	UNP P0DTC2
B	1244	GLU	-	expression tag	UNP P0DTC2
B	1245	TRP	-	expression tag	UNP P0DTC2
B	1246	VAL	-	expression tag	UNP P0DTC2
B	1247	LEU	-	expression tag	UNP P0DTC2
B	1248	LEU	-	expression tag	UNP P0DTC2
B	1249	SER	-	expression tag	UNP P0DTC2
B	1250	THR	-	expression tag	UNP P0DTC2
B	1251	PHE	-	expression tag	UNP P0DTC2
B	1252	LEU	-	expression tag	UNP P0DTC2
B	1253	GLY	-	expression tag	UNP P0DTC2
B	1254	HIS	-	expression tag	UNP P0DTC2
B	1255	HIS	-	expression tag	UNP P0DTC2
B	1256	HIS	-	expression tag	UNP P0DTC2
B	1257	HIS	-	expression tag	UNP P0DTC2
B	1258	HIS	-	expression tag	UNP P0DTC2
B	1259	HIS	-	expression tag	UNP P0DTC2
C	?	-	ARG	deletion	UNP P0DTC2
C	?	-	ARG	deletion	UNP P0DTC2
C	?	-	ALA	deletion	UNP P0DTC2
C	685	ALA	ARG	engineered mutation	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	1214	SER	-	expression tag	UNP P0DTC2
C	1215	GLY	-	expression tag	UNP P0DTC2
C	1216	ARG	-	expression tag	UNP P0DTC2
C	1217	LEU	-	expression tag	UNP P0DTC2
C	1218	VAL	-	expression tag	UNP P0DTC2
C	1219	PRO	-	expression tag	UNP P0DTC2
C	1220	ARG	-	expression tag	UNP P0DTC2
C	1221	GLY	-	expression tag	UNP P0DTC2
C	1222	SER	-	expression tag	UNP P0DTC2
C	1223	PRO	-	expression tag	UNP P0DTC2
C	1224	GLY	-	expression tag	UNP P0DTC2
C	1225	SER	-	expression tag	UNP P0DTC2
C	1226	GLY	-	expression tag	UNP P0DTC2
C	1227	TYR	-	expression tag	UNP P0DTC2
C	1228	ILE	-	expression tag	UNP P0DTC2
C	1229	PRO	-	expression tag	UNP P0DTC2
C	1230	GLU	-	expression tag	UNP P0DTC2
C	1231	ALA	-	expression tag	UNP P0DTC2
C	1232	PRO	-	expression tag	UNP P0DTC2
C	1233	ARG	-	expression tag	UNP P0DTC2
C	1234	ASP	-	expression tag	UNP P0DTC2
C	1235	GLY	-	expression tag	UNP P0DTC2
C	1236	GLN	-	expression tag	UNP P0DTC2
C	1237	ALA	-	expression tag	UNP P0DTC2
C	1238	TYR	-	expression tag	UNP P0DTC2
C	1239	VAL	-	expression tag	UNP P0DTC2
C	1240	ARG	-	expression tag	UNP P0DTC2
C	1241	LYS	-	expression tag	UNP P0DTC2
C	1242	ASP	-	expression tag	UNP P0DTC2
C	1243	GLY	-	expression tag	UNP P0DTC2
C	1244	GLU	-	expression tag	UNP P0DTC2
C	1245	TRP	-	expression tag	UNP P0DTC2
C	1246	VAL	-	expression tag	UNP P0DTC2
C	1247	LEU	-	expression tag	UNP P0DTC2
C	1248	LEU	-	expression tag	UNP P0DTC2
C	1249	SER	-	expression tag	UNP P0DTC2
C	1250	THR	-	expression tag	UNP P0DTC2
C	1251	PHE	-	expression tag	UNP P0DTC2
C	1252	LEU	-	expression tag	UNP P0DTC2
C	1253	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1254	HIS	-	expression tag	UNP P0DTC2
C	1255	HIS	-	expression tag	UNP P0DTC2
C	1256	HIS	-	expression tag	UNP P0DTC2
C	1257	HIS	-	expression tag	UNP P0DTC2
C	1258	HIS	-	expression tag	UNP P0DTC2
C	1259	HIS	-	expression tag	UNP P0DTC2

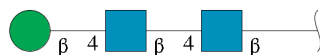
- Molecule 2 is a protein called 2B04 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	119	Total	C	N	O	S	0	0
			926	587	158	177	4		
2	I	119	Total	C	N	O	S	0	0
			926	587	158	177	4		

- Molecule 3 is a protein called 2B04 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	109	Total	C	N	O	S	0	0
			812	511	138	161	2		
3	M	109	Total	C	N	O	S	0	0
			812	511	138	161	2		

- Molecule 4 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
4	D	3	Total	C	N	O		0	0
			39	22	2	15			
4	E	3	Total	C	N	O		0	0
			39	22	2	15			
4	S	3	Total	C	N	O		0	0
			39	22	2	15			
4	T	3	Total	C	N	O		0	0
			39	22	2	15			
4	V	3	Total	C	N	O		0	0
			39	22	2	15			

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Mol	Chain	Residues	Atoms				AltConf	Trace
4	W	3	Total	C	N	O	0	0
			39	22	2	15		
4	a	3	Total	C	N	O	0	0
			39	22	2	15		
4	e	3	Total	C	N	O	0	0
			39	22	2	15		
4	h	3	Total	C	N	O	0	0
			39	22	2	15		
4	i	3	Total	C	N	O	0	0
			39	22	2	15		
4	j	3	Total	C	N	O	0	0
			39	22	2	15		
4	m	3	Total	C	N	O	0	0
			39	22	2	15		
4	u	3	Total	C	N	O	0	0
			39	22	2	15		
4	v	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 5 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
5	F	2	Total	C	N	O	0	0
			28	16	2	10		
5	G	2	Total	C	N	O	0	0
			28	16	2	10		
5	K	2	Total	C	N	O	0	0
			28	16	2	10		
5	N	2	Total	C	N	O	0	0
			28	16	2	10		
5	O	2	Total	C	N	O	0	0
			28	16	2	10		
5	Q	2	Total	C	N	O	0	0
			28	16	2	10		
5	R	2	Total	C	N	O	0	0
			28	16	2	10		
5	X	2	Total	C	N	O	0	0
			28	16	2	10		

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Mol	Chain	Residues	Atoms				AltConf	Trace
5	Y	2	Total	C	N	O	0	0
			28	16	2	10		
5	Z	2	Total	C	N	O	0	0
			28	16	2	10		
5	c	2	Total	C	N	O	0	0
			28	16	2	10		
5	d	2	Total	C	N	O	0	0
			28	16	2	10		
5	f	2	Total	C	N	O	0	0
			28	16	2	10		
5	g	2	Total	C	N	O	0	0
			28	16	2	10		
5	k	2	Total	C	N	O	0	0
			28	16	2	10		
5	l	2	Total	C	N	O	0	0
			28	16	2	10		
5	o	2	Total	C	N	O	0	0
			28	16	2	10		
5	p	2	Total	C	N	O	0	0
			28	16	2	10		
5	q	2	Total	C	N	O	0	0
			28	16	2	10		
5	s	2	Total	C	N	O	0	0
			28	16	2	10		
5	t	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 6 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
6	J	2	Total	C	N	O	0	0
			24	14	1	9		
6	b	2	Total	C	N	O	0	0
			24	14	1	9		
6	n	2	Total	C	N	O	0	0
			24	14	1	9		

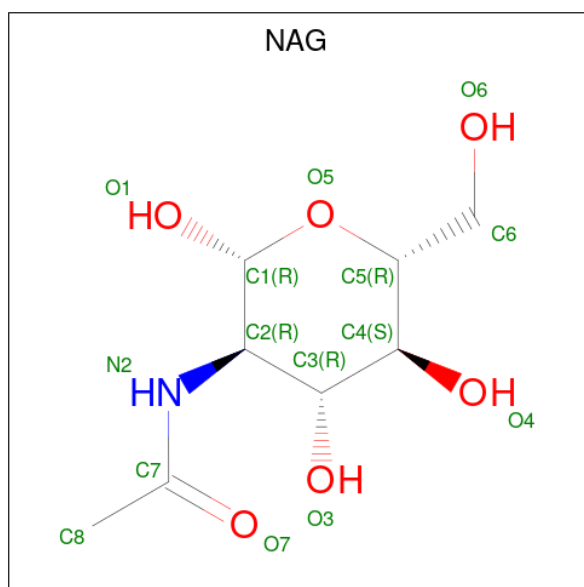
- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranos

e-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
7	P	4	Total	C	N	O	0	0
			50	28	2	20		
7	U	4	Total	C	N	O	0	0
			50	28	2	20		
7	r	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).

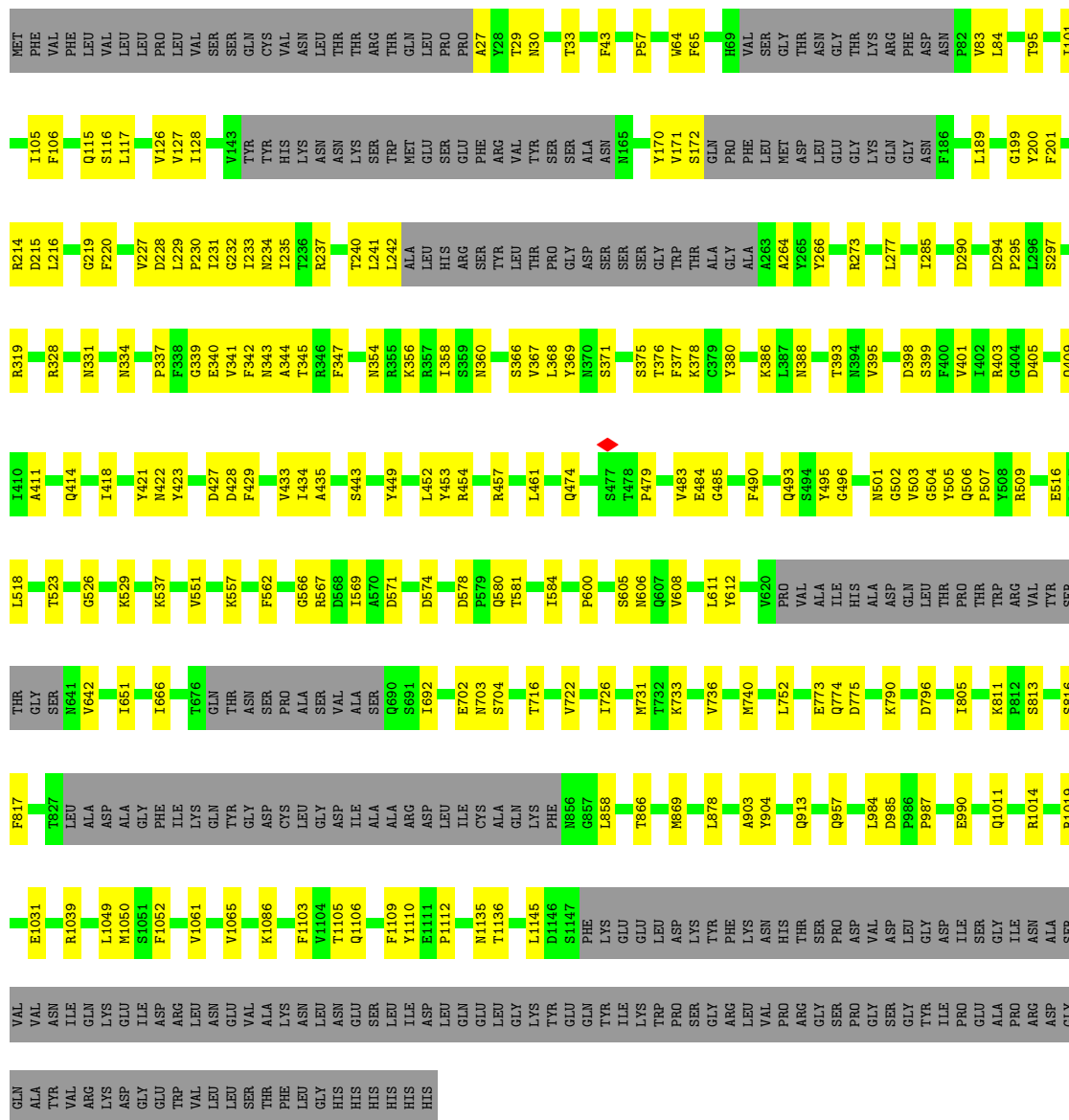


Mol	Chain	Residues	Atoms				AltConf
8	A	1	Total	C	N	O	0
			14	8	1	5	
8	B	1	Total	C	N	O	0
			14	8	1	5	
8	C	1	Total	C	N	O	0
			14	8	1	5	

TYR
ILE
PRO
GLU
ALA
PRO
ARG
ASP
GLY
GLN
ALA
TYR
VAL
ARG
LYS
ASP
GLY
GLU
TRP
VAL
LEU
GLY
HIS
HIS
HIS
HIS
HIS

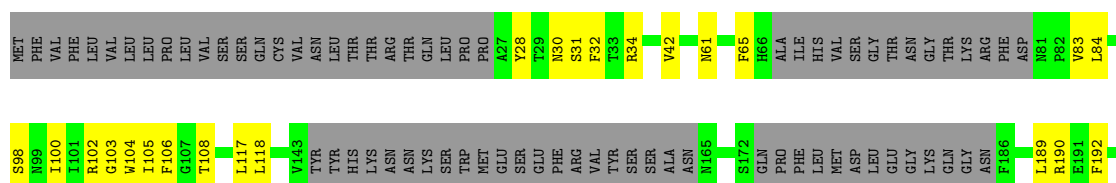
• Molecule 1: Spike glycoprotein

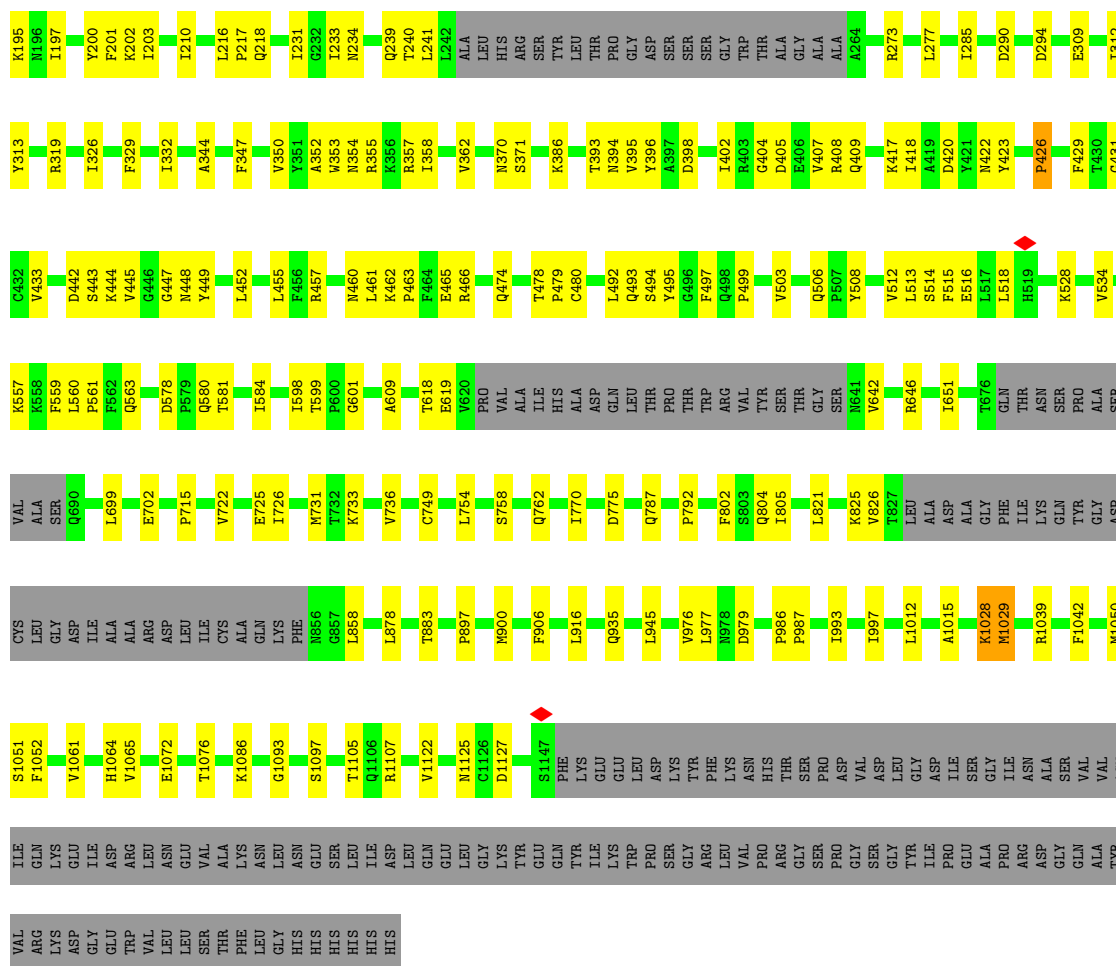
Chain B:  63% 17% 21%



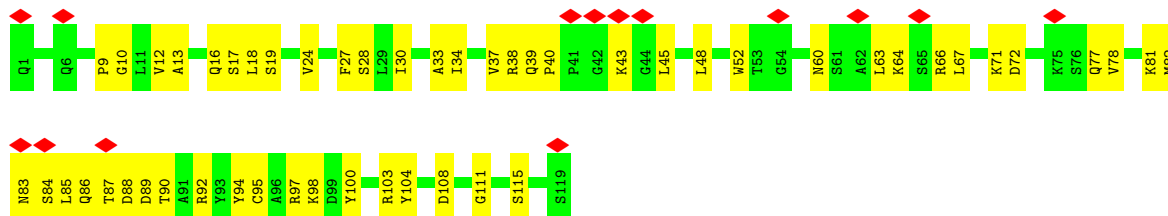
• Molecule 1: Spike glycoprotein

Chain C:  63% 16% 21%





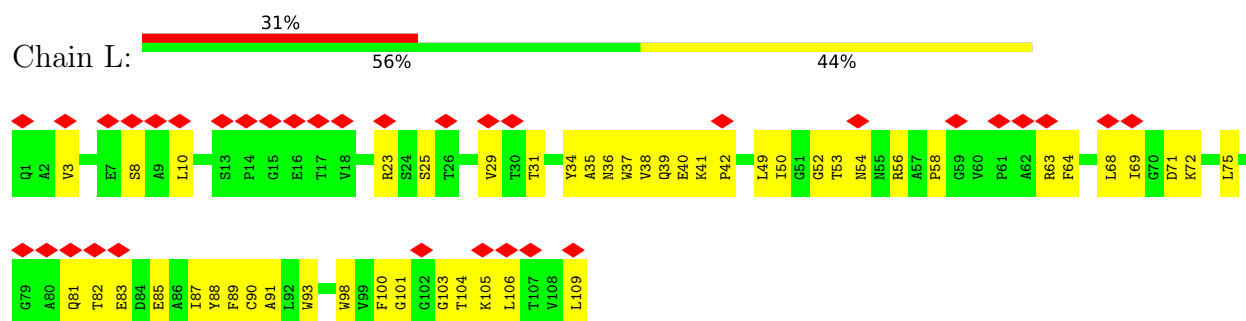
• Molecule 2: 2B04 heavy chain



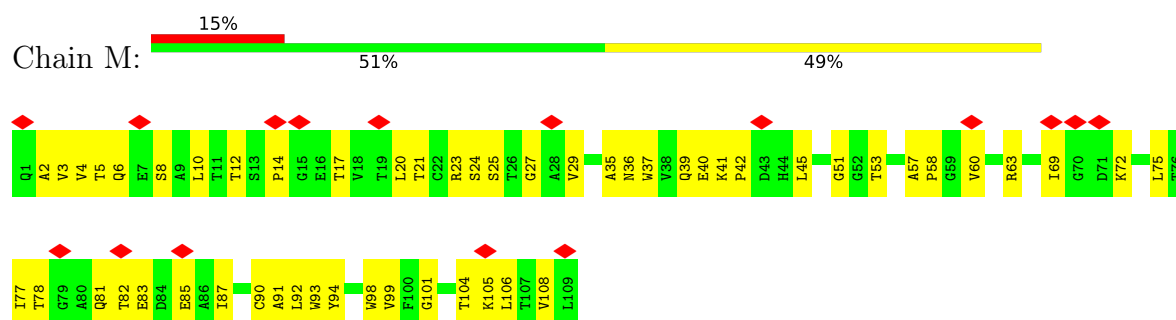
• Molecule 2: 2B04 heavy chain



- Molecule 3: 2B04 light chain



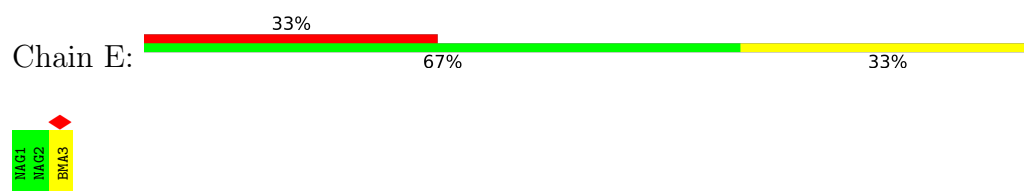
- Molecule 3: 2B04 light chain



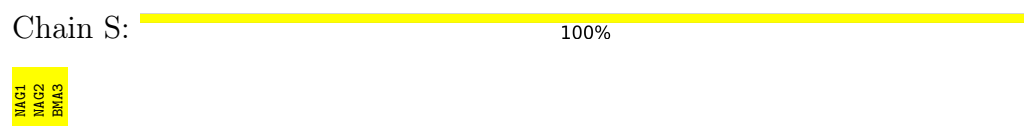
- Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



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

Chain T:  100%

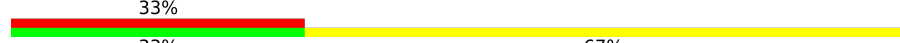


- Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:  33% 67%



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

Chain W:  33% 33% 67%



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

Chain a:  33% 67% 33%



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

Chain e:  33% 67%



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

Chain h:  33% 100%



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

Chain i:  100%



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



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



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



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



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  100%

NAG1
NAG2

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:  50% 100%

♦
NAG1
NAG2

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:  50% 50%

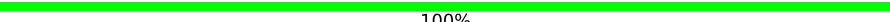
NAG1
NAG2

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:  100%

NAG1
NAG2

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:  100%

NAG1
NAG2

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:  50% 50%

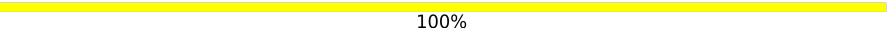
NAG1
NAG2

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:  50% 50%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:  100%

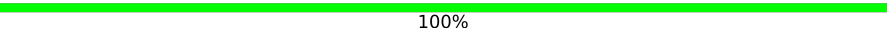


- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c:  50% 50% 50%

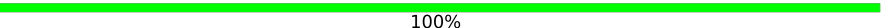


- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d:  100%

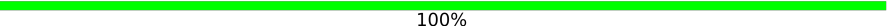


- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain f:  100%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain g:  100%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain k:  50% 50%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain l:  100%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain o:  100%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain p:  50% 50%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain q:  100%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain s:  50% 50%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain t:  100%



- Molecule 6: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 7: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 7: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 7: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	162281	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	67	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.967	Depositor
Minimum map value	-1.669	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.076	Depositor
Recommended contour level	0.25	Depositor
Map size (Å)	330.0, 330.0, 330.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	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: MAN, FUC, BMA, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.27	0/7011	0.42	0/9572
1	B	0.27	0/7822	0.43	0/10659
1	C	0.27	0/7796	0.45	1/10624 (0.0%)
2	H	0.12	0/948	0.37	0/1285
2	I	0.14	0/948	0.43	0/1285
3	L	0.13	0/830	0.37	0/1136
3	M	0.12	0/830	0.39	0/1136
All	All	0.25	0/26185	0.43	1/35697 (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	426	PRO	CB-CA-C	-5.18	104.20	110.98

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	6876	0	6311	105	0
1	B	7649	0	7396	157	0
1	C	7623	0	7365	143	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	926	0	908	47	0
2	I	926	0	908	53	0
3	L	812	0	786	33	0
3	M	812	0	786	44	0
4	D	39	0	34	0	0
4	E	39	0	34	0	0
4	S	39	0	34	0	0
4	T	39	0	34	0	0
4	V	39	0	34	0	0
4	W	39	0	34	1	0
4	a	39	0	34	1	0
4	e	39	0	34	1	0
4	h	39	0	34	0	0
4	i	39	0	34	0	0
4	j	39	0	34	0	0
4	m	39	0	34	0	0
4	u	39	0	34	0	0
4	v	39	0	34	2	0
5	F	28	0	25	0	0
5	G	28	0	25	0	0
5	K	28	0	25	1	0
5	N	28	0	25	0	0
5	O	28	0	25	1	0
5	Q	28	0	25	0	0
5	R	28	0	25	0	0
5	X	28	0	25	0	0
5	Y	28	0	25	1	0
5	Z	28	0	25	2	0
5	c	28	0	25	0	0
5	d	28	0	25	0	0
5	f	28	0	25	0	0
5	g	28	0	25	0	0
5	k	28	0	25	1	0
5	l	28	0	25	2	0
5	o	28	0	25	0	0
5	p	28	0	25	2	0
5	q	28	0	25	0	0
5	s	28	0	25	0	0
5	t	28	0	25	0	0
6	J	24	0	22	0	0
6	b	24	0	22	0	0
6	n	24	0	22	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	P	50	0	43	0	0
7	U	50	0	43	0	0
7	r	50	0	43	0	0
8	A	14	0	13	0	0
8	B	14	0	13	0	0
8	C	14	0	13	0	0
All	All	27022	0	25695	542	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 10.

All (542) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:449:TYR:CG	2:I:28:SER:HB3	1.97	0.99
1:B:449:TYR:HB3	2:H:28:SER:HB3	1.47	0.93
2:H:9:PRO:HG2	2:H:18:LEU:HD11	1.62	0.81
1:B:378:LYS:NZ	1:B:380:TYR:OH	2.15	0.79
1:B:105:ILE:HG13	1:B:241:LEU:HD11	1.65	0.78
3:L:40:GLU:HB3	3:L:87:ILE:HB	1.66	0.77
1:C:733:LYS:NZ	1:C:775:ASP:OD2	2.17	0.77
1:B:752:LEU:HD21	1:B:990:GLU:HG3	1.66	0.77
3:M:8:SER:HA	3:M:104:THR:HA	1.68	0.76
1:B:557:LYS:NZ	1:B:574:ASP:OD2	2.21	0.73
1:B:811:LYS:HD3	1:B:813:SER:H	1.53	0.73
2:I:6:GLN:NE2	2:I:93:TYR:O	2.19	0.73
1:A:726:ILE:HG12	1:A:1061:VAL:HG22	1.71	0.73
1:B:337:PRO:O	1:B:340:GLU:HG3	1.89	0.72
1:C:642:VAL:HG12	1:C:651:ILE:HG12	1.71	0.72
1:B:29:THR:HG22	1:B:30:ASN:H	1.53	0.72
1:C:449:TYR:CB	2:I:28:SER:HB3	2.20	0.71
1:C:108:THR:OG1	1:C:234:ASN:O	2.09	0.71
1:C:357:ARG:HE	1:C:396:TYR:HE1	1.36	0.71
2:I:66:ARG:HB3	2:I:83:ASN:HD21	1.55	0.71
1:C:599:THR:HG22	1:C:601:GLY:H	1.55	0.71
1:A:707:TYR:HB3	1:C:792:PRO:HG3	1.72	0.70
2:I:97:ARG:NH2	2:I:108:ASP:OD2	2.23	0.70
1:B:358:ILE:HB	1:B:395:VAL:HG13	1.73	0.70
3:M:41:LYS:HE3	3:M:42:PRO:HD2	1.73	0.70
1:B:1011:GLN:OE1	1:B:1014:ARG:NH1	2.24	0.70
3:L:10:LEU:HG	3:L:106:LEU:HD13	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:345:THR:O	1:B:509:ARG:NH2	2.25	0.70
3:L:3:VAL:HG12	3:L:25:SER:HB2	1.73	0.70
3:L:36:ASN:HB2	3:L:91:ALA:HB3	1.73	0.69
1:A:557:LYS:NZ	1:A:574:ASP:OD1	2.24	0.69
1:B:449:TYR:CB	2:H:28:SER:HB3	2.23	0.69
2:I:38:ARG:HB2	2:I:48:LEU:HD11	1.75	0.69
2:I:80:LEU:HD21	2:I:82:MET:HE3	1.75	0.68
3:M:36:ASN:HB2	3:M:91:ALA:HB3	1.74	0.68
3:L:8:SER:HA	3:L:104:THR:HA	1.75	0.68
1:C:105:ILE:HD12	1:C:118:LEU:HD22	1.75	0.68
3:M:21:THR:O	3:M:23:ARG:NH1	2.27	0.68
1:B:128:ILE:HG21	1:B:229:LEU:HD21	1.75	0.67
1:C:449:TYR:CD2	2:I:28:SER:HB3	2.28	0.67
3:M:12:THR:HG22	3:M:106:LEU:HD11	1.75	0.67
2:H:66:ARG:HG2	2:H:83:ASN:HD21	1.59	0.67
1:A:1135:ASN:OD1	1:A:1136:THR:N	2.27	0.67
1:A:210:ILE:HD11	1:A:217:PRO:HG3	1.76	0.67
1:B:484:GLU:HB2	2:H:52:TRP:CD2	2.29	0.67
2:I:29:LEU:HD12	2:I:73:ASN:HA	1.76	0.67
1:C:445:VAL:HA	1:C:499:PRO:HG3	1.77	0.66
1:A:984:LEU:O	1:B:386:LYS:NZ	2.28	0.66
1:B:740:MET:SD	1:C:319:ARG:NH1	2.69	0.66
1:B:985:ASP:HB3	1:B:987:PRO:HD2	1.78	0.66
3:M:40:GLU:HB3	3:M:87:ILE:HB	1.77	0.66
1:B:341:VAL:HG13	1:B:342:PHE:HD1	1.61	0.65
1:A:100:ILE:HD12	1:A:100:ILE:H	1.61	0.65
1:A:200:TYR:HE2	1:A:228:ASP:HB3	1.61	0.65
1:B:421:TYR:HA	1:B:461:LEU:HD13	1.80	0.64
3:M:63:ARG:NH1	3:M:78:THR:O	2.31	0.64
1:B:27:ALA:HB3	1:B:64:TRP:HE3	1.63	0.64
2:H:17:SER:OG	2:H:81:LYS:NZ	2.22	0.63
3:L:39:GLN:HB2	3:L:49:LEU:HD11	1.80	0.63
1:B:502:GLY:O	1:B:506:GLN:NE2	2.25	0.63
1:C:646:ARG:NH1	1:C:646:ARG:O	2.26	0.63
2:H:39:GLN:NE2	2:H:43:LYS:O	2.26	0.63
2:H:95:CYS:O	2:H:111:GLY:N	2.31	0.63
3:L:56:ARG:NE	3:L:64:PHE:O	2.31	0.63
1:C:494:SER:HB3	2:I:30:ILE:HB	1.80	0.63
3:L:34:TYR:HD1	3:L:52:GLY:HA2	1.61	0.63
1:A:738:CYS:SG	1:A:739:THR:N	2.72	0.63
1:B:127:VAL:HG22	1:B:171:VAL:HG22	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:490:PHE:O	1:B:493:GLN:NE2	2.32	0.62
1:B:215:ASP:HA	1:B:266:TYR:OH	1.99	0.62
1:B:790:LYS:NZ	1:C:702:GLU:OE2	2.31	0.62
2:I:86:GLN:HE22	2:I:88:ASP:HB3	1.63	0.62
3:M:36:ASN:HD22	3:M:51:GLY:HA2	1.64	0.62
1:C:195:LYS:HD2	1:C:197:ILE:HD11	1.82	0.62
1:C:444:LYS:NZ	1:C:447:GLY:O	2.31	0.61
1:A:504:GLY:HA2	3:L:71:ASP:OD1	2.01	0.61
2:H:64:LYS:HG2	2:H:67:LEU:HD23	1.82	0.61
3:L:63:ARG:NH2	3:L:83:GLU:OE1	2.33	0.61
3:L:35:ALA:HB3	3:L:53:THR:HA	1.83	0.61
1:B:360:ASN:H	1:B:523:THR:HG23	1.66	0.61
1:C:239:GLN:NE2	1:C:240:THR:O	2.34	0.60
1:C:273:ARG:NH1	1:C:290:ASP:OD2	2.33	0.60
2:I:112:GLN:NE2	2:I:113:GLY:O	2.33	0.60
1:C:393:THR:N	1:C:516:GLU:OE1	2.29	0.60
1:B:703:ASN:OD1	1:B:704:SER:N	2.35	0.60
2:H:104:TYR:HE2	2:H:108:ASP:HA	1.67	0.60
1:A:393:THR:HA	1:A:522:ALA:HA	1.83	0.60
2:I:50:VAL:HG21	2:I:98:LYS:HE2	1.84	0.60
1:A:619:GLU:OE1	1:A:619:GLU:N	2.34	0.59
1:B:1050:MET:HE2	1:B:1052:PHE:CZ	2.37	0.59
1:C:460:ASN:OD1	1:C:461:LEU:N	2.35	0.59
1:B:642:VAL:HG22	1:B:651:ILE:HG22	1.84	0.59
1:A:403:ARG:HA	1:A:507:PRO:HA	1.83	0.59
1:A:707:TYR:HB2	1:C:883:THR:HG23	1.85	0.59
1:C:431:GLY:HA2	1:C:515:PHE:CD2	2.38	0.59
3:M:23:ARG:HG3	3:M:72:LYS:HG3	1.82	0.59
1:A:36:VAL:HG21	1:A:220:PHE:CZ	2.37	0.59
2:I:71:LYS:HA	2:I:78:VAL:HA	1.84	0.59
3:L:40:GLU:HB2	3:L:89:PHE:HE1	1.66	0.59
1:B:57:PRO:HG3	1:B:273:ARG:HD2	1.82	0.59
2:H:103:ARG:HD2	2:H:104:TYR:N	2.18	0.59
3:M:82:THR:OG1	3:M:83:GLU:OE2	2.20	0.59
1:A:557:LYS:HB2	1:A:584:ILE:HD13	1.85	0.59
3:M:29:VAL:HB	3:M:92:LEU:HD21	1.85	0.59
2:H:60:ASN:HB3	2:H:63:LEU:HB2	1.84	0.58
1:B:367:VAL:HG23	1:B:368:LEU:HD12	1.86	0.58
5:K:1:NAG:H5	5:K:2:NAG:H83	1.83	0.58
1:A:105:ILE:HD11	1:A:241:LEU:HD12	1.86	0.58
1:B:1105:THR:HG22	1:B:1112:PRO:HA	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:516:GLU:OE2	1:C:516:GLU:N	2.36	0.58
1:A:43:PHE:HB3	1:B:566:GLY:HA2	1.86	0.58
1:C:104:TRP:HB3	1:C:106:PHE:CE2	2.39	0.58
1:B:101:ILE:HD12	1:B:242:LEU:HA	1.85	0.57
1:A:226:LEU:HD23	1:A:227:VAL:HG23	1.86	0.57
1:A:741:TYR:CE1	1:A:966:LEU:HD11	2.39	0.57
1:A:1102:TRP:CD1	1:A:1135:ASN:HD22	2.22	0.57
1:A:1125:ASN:ND2	1:A:1127:ASP:OD1	2.37	0.57
1:B:340:GLU:OE2	1:B:356:LYS:NZ	2.25	0.57
2:H:86:GLN:HE22	2:H:88:ASP:HB2	1.69	0.57
3:M:36:ASN:ND2	3:M:51:GLY:HA2	2.19	0.57
3:M:41:LYS:HB2	3:M:45:LEU:HB2	1.87	0.57
3:L:34:TYR:CD1	3:L:52:GLY:HA2	2.38	0.57
1:C:462:LYS:N	1:C:465:GLU:OE1	2.38	0.57
2:H:64:LYS:HE3	2:H:82:MET:HE1	1.86	0.57
1:B:216:LEU:H	1:B:216:LEU:HD12	1.69	0.57
1:A:106:PHE:HB3	1:A:235:ILE:HD12	1.85	0.57
2:I:13:ALA:H	2:I:16:GLN:HE22	1.52	0.57
1:A:676:THR:HA	1:A:690:GLN:HA	1.88	0.56
1:C:405:ASP:O	1:C:408:ARG:NH1	2.39	0.56
1:C:993:ILE:O	1:C:997:ILE:HG12	2.05	0.56
1:B:64:TRP:CD1	1:B:266:TYR:CE1	2.93	0.56
1:B:295:PRO:HB2	1:B:608:VAL:HG21	1.87	0.56
1:C:726:ILE:HG12	1:C:1061:VAL:HG22	1.86	0.56
1:C:802:PHE:HD1	1:C:805:ILE:HD11	1.71	0.56
1:A:406:GLU:O	1:A:410:ILE:N	2.39	0.56
1:C:804:GLN:NE2	1:C:935:GLN:OE1	2.38	0.56
1:B:200:TYR:OH	1:C:394:ASN:ND2	2.38	0.56
1:B:452:LEU:HD21	2:H:30:ILE:HG21	1.87	0.56
3:M:90:CYS:O	3:M:101:GLY:N	2.39	0.56
1:C:457:ARG:NH1	1:C:460:ASN:O	2.38	0.56
1:C:578:ASP:OD1	1:C:581:THR:N	2.36	0.56
1:A:1098:ASN:OD1	1:A:1099:GLY:N	2.40	0.56
1:B:331:ASN:HB3	5:Z:1:NAG:O5	2.06	0.55
1:A:1145:LEU:HA	1:B:1145:LEU:HD21	1.87	0.55
1:B:230:PRO:HB2	1:C:357:ARG:HH11	1.71	0.55
2:H:38:ARG:HB2	2:H:48:LEU:HD11	1.88	0.55
2:H:72:ASP:N	2:H:77:GLN:O	2.39	0.55
3:M:6:GLN:HA	3:M:23:ARG:HH12	1.72	0.55
1:B:339:GLY:HA2	4:a:1:NAG:H83	1.89	0.55
2:H:63:LEU:HG	2:H:67:LEU:HD21	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:90:THR:HB	2:I:118:VAL:HG12	1.88	0.55
3:M:29:VAL:HG13	3:M:72:LYS:HD2	1.89	0.55
5:p:1:NAG:HO6	5:p:2:NAG:HO6	1.53	0.55
1:C:350:VAL:HG11	1:C:418:ILE:HD11	1.89	0.54
4:W:2:NAG:HN2	4:W:3:BMA:H2	1.72	0.54
1:A:790:LYS:NZ	1:B:702:GLU:OE2	2.36	0.54
1:B:401:VAL:HG22	1:B:509:ARG:HG2	1.90	0.54
1:C:28:TYR:HB3	1:C:61:ASN:HD21	1.73	0.54
1:C:1076:THR:HG23	1:C:1097:SER:HB3	1.89	0.54
1:B:773:GLU:OE2	1:B:1019:ARG:NH1	2.34	0.54
1:C:358:ILE:HB	1:C:395:VAL:HG23	1.89	0.54
1:A:354:ASN:O	1:A:398:ASP:HA	2.07	0.54
2:H:97:ARG:NH2	2:H:108:ASP:OD2	2.37	0.54
1:B:380:TYR:HD2	1:B:429:PHE:HD2	1.55	0.54
1:A:532:ASN:OD1	1:A:533:LEU:N	2.39	0.53
1:B:805:ILE:HG13	1:B:878:LEU:HD21	1.90	0.53
1:B:398:ASP:OD2	1:B:423:TYR:OH	2.25	0.53
3:M:4:VAL:HG13	3:M:101:GLY:HA2	1.91	0.53
1:C:370:ASN:OD1	1:C:371:SER:N	2.41	0.53
1:C:442:ASP:O	1:C:448:ASN:ND2	2.33	0.53
3:M:35:ALA:HB3	3:M:53:THR:HA	1.91	0.53
1:A:705:VAL:HG13	1:C:883:THR:HG21	1.91	0.53
1:A:1098:ASN:CG	1:A:1101:HIS:H	2.17	0.53
3:L:93:TRP:HB2	3:L:98:TRP:CH2	2.44	0.53
1:A:1098:ASN:OD1	1:A:1101:HIS:N	2.35	0.53
1:B:366:SER:HB2	1:B:388:ASN:HD21	1.74	0.53
1:C:494:SER:CB	2:I:30:ILE:HB	2.38	0.53
1:C:722:VAL:HG22	1:C:1065:VAL:HG22	1.90	0.53
1:C:494:SER:HB2	2:I:30:ILE:HG21	1.91	0.52
2:H:71:LYS:HA	2:H:78:VAL:HA	1.89	0.52
2:I:15:SER:HA	2:I:85:LEU:H	1.74	0.52
1:B:294:ASP:N	1:B:294:ASP:OD1	2.40	0.52
1:B:990:GLU:N	1:B:990:GLU:OE1	2.42	0.52
1:C:1125:ASN:ND2	1:C:1127:ASP:OD1	2.42	0.52
1:C:1051:SER:OG	1:C:1064:HIS:ND1	2.39	0.52
1:B:474:GLN:HG3	1:B:479:PRO:HA	1.91	0.52
5:p:1:NAG:O6	5:p:2:NAG:O6	2.26	0.52
1:A:353:TRP:HA	1:A:399:SER:O	2.09	0.52
3:M:37:TRP:CE2	3:M:75:LEU:HB2	2.45	0.52
1:B:427:ASP:OD1	1:B:428:ASP:N	2.42	0.52
1:C:294:ASP:OD1	1:C:294:ASP:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1031:GLU:OE2	1:C:1039:ARG:NH2	2.43	0.52
1:A:542:ASN:HA	1:A:546:LEU:O	2.10	0.52
1:C:493:GLN:HG3	2:I:101:TYR:CZ	2.45	0.52
1:B:393:THR:OG1	1:B:516:GLU:OE1	2.27	0.51
1:C:906:PHE:CD2	1:C:916:LEU:HB2	2.45	0.51
3:M:57:ALA:HB3	3:M:60:VAL:HB	1.92	0.51
1:A:578:ASP:HB3	1:A:581:THR:O	2.11	0.51
1:B:600:PRO:HD3	1:B:692:ILE:HD11	1.92	0.51
1:C:452:LEU:HD23	1:C:492:LEU:HD21	1.91	0.51
1:C:503:VAL:HA	1:C:506:GLN:HG2	1.91	0.51
1:A:811:LYS:NZ	1:A:820:ASP:OD2	2.32	0.51
1:A:986:PRO:HB2	1:A:987:PRO:HD3	1.93	0.51
2:I:53:THR:O	2:I:71:LYS:NZ	2.43	0.51
2:I:72:ASP:N	2:I:77:GLN:O	2.37	0.51
1:B:344:ALA:HB3	1:B:347:PHE:HE1	1.75	0.51
1:B:484:GLU:OE1	2:H:52:TRP:HB3	2.10	0.51
1:C:326:ILE:HD11	1:C:534:VAL:HG22	1.92	0.51
1:C:770:ILE:HD11	1:C:1012:LEU:HD23	1.92	0.51
1:C:1093:GLY:HA3	1:C:1105:THR:O	2.09	0.51
1:C:402:ILE:HD11	1:C:407:VAL:HG12	1.92	0.51
3:M:24:SER:HG	3:M:94:TYR:HH	1.50	0.51
1:B:1050:MET:HE2	1:B:1052:PHE:CE1	2.46	0.51
2:I:12:VAL:N	2:I:117:THR:O	2.42	0.51
1:B:277:LEU:HD23	1:B:285:ILE:HD13	1.93	0.51
1:B:866:THR:H	1:B:869:MET:HE3	1.76	0.51
1:C:474:GLN:NE2	1:C:478:THR:O	2.42	0.51
1:B:328:ARG:HH21	1:B:580:GLN:HB2	1.76	0.51
1:B:904:TYR:CE1	1:C:1107:ARG:HD3	2.45	0.51
1:B:984:LEU:O	1:C:386:LYS:NZ	2.32	0.51
1:C:197:ILE:HB	1:C:202:LYS:HE3	1.92	0.51
2:I:90:THR:HB	2:I:118:VAL:H	1.76	0.51
1:A:1115:ILE:HG22	1:A:1137:VAL:HG13	1.92	0.50
1:B:816:SER:OG	1:B:817:PHE:N	2.43	0.50
2:H:33:ALA:HB3	2:H:98:LYS:HE3	1.93	0.50
3:M:10:LEU:N	3:M:105:LYS:O	2.39	0.50
1:A:131:CYS:HB2	1:A:133:PHE:CE2	2.45	0.50
1:B:578:ASP:HB3	1:B:581:THR:O	2.10	0.50
1:B:233:ILE:HG23	1:B:235:ILE:HD11	1.93	0.50
1:C:559:PHE:CZ	1:C:584:ILE:HD12	2.46	0.50
2:H:13:ALA:H	2:H:16:GLN:NE2	2.09	0.50
1:C:98:SER:HB3	1:C:100:ILE:HG12	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:12:VAL:HG22	2:H:18:LEU:HD13	1.94	0.49
1:B:233:ILE:HG12	1:B:234:ASN:N	2.27	0.49
5:Z:1:NAG:O3	5:Z:2:NAG:H2	2.12	0.49
1:A:1080:ALA:O	1:A:1132:ILE:HG13	2.11	0.49
3:L:31:THR:HG23	3:L:53:THR:HB	1.94	0.49
1:B:214:ARG:NH1	1:B:214:ARG:HA	2.27	0.49
1:B:612:TYR:HE1	1:B:651:ILE:HD11	1.77	0.49
1:A:731:MET:HG2	1:A:1018:ILE:HG13	1.95	0.49
1:B:454:ARG:HH22	1:B:457:ARG:HG3	1.78	0.49
3:M:29:VAL:HG22	3:M:72:LYS:HA	1.94	0.49
1:B:483:VAL:HG12	1:B:485:GLY:H	1.77	0.49
1:A:323:THR:HG1	1:A:324:GLU:CD	2.19	0.49
1:A:902:MET:HE1	1:A:1050:MET:SD	2.53	0.49
1:C:493:GLN:HG3	2:I:101:TYR:OH	2.13	0.49
1:B:65:PHE:CE1	1:B:84:LEU:HD21	2.47	0.49
1:C:1050:MET:HE2	1:C:1052:PHE:CE1	2.48	0.49
1:A:424:LYS:O	1:A:464:PHE:N	2.36	0.49
1:C:749:CYS:SG	1:C:997:ILE:HD11	2.53	0.49
2:I:81:LYS:O	2:I:82:MET:HE2	2.13	0.49
3:L:90:CYS:O	3:L:101:GLY:N	2.46	0.49
1:A:1077:THR:OG1	1:C:900:MET:HE1	2.12	0.49
3:M:5:THR:O	3:M:23:ARG:NH1	2.46	0.49
2:H:34:ILE:HD13	2:H:97:ARG:HA	1.94	0.48
2:I:95:CYS:O	2:I:111:GLY:N	2.46	0.48
1:A:676:THR:HG22	1:A:690:GLN:HG3	1.95	0.48
1:B:126:VAL:HG22	1:B:172:SER:HB3	1.95	0.48
1:C:409:GLN:OE1	1:C:418:ILE:HG22	2.14	0.48
3:L:81:GLN:HG2	3:L:109:LEU:HD21	1.95	0.48
1:B:567:ARG:HG2	1:B:571:ASP:HA	1.94	0.48
2:H:103:ARG:NH2	3:L:58:PRO:HB3	2.28	0.48
1:A:97:LYS:NZ	1:A:187:LYS:H	2.10	0.48
1:A:642:VAL:HG12	1:A:651:ILE:HG12	1.96	0.48
3:M:93:TRP:HB2	3:M:98:TRP:CH2	2.49	0.48
5:l:1:NAG:O3	5:l:2:NAG:H2	2.14	0.48
1:B:344:ALA:O	1:B:509:ARG:NH1	2.30	0.48
2:H:66:ARG:HH21	2:H:84:SER:HB3	1.77	0.48
1:A:97:LYS:HZ1	1:A:188:ASN:H	1.60	0.48
1:A:131:CYS:HB2	1:A:133:PHE:CD2	2.49	0.48
1:A:355:ARG:HA	1:A:397:ALA:O	2.13	0.48
2:I:37:VAL:HG23	2:I:94:TYR:HB2	1.96	0.48
1:A:281:GLU:N	1:A:281:GLU:OE1	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:3:VAL:O	3:M:25:SER:N	2.47	0.48
1:B:611:LEU:HD22	1:B:666:ILE:HG23	1.96	0.47
1:A:294:ASP:OD1	1:A:294:ASP:N	2.47	0.47
3:M:75:LEU:HD21	3:M:77:ILE:HD11	1.95	0.47
1:A:130:VAL:HG12	1:A:168:PHE:HB3	1.95	0.47
1:C:344:ALA:HB3	1:C:347:PHE:CE1	2.49	0.47
2:I:2:VAL:HG21	2:I:109:TYR:CD1	2.49	0.47
3:L:37:TRP:CE2	3:L:75:LEU:HB2	2.50	0.47
2:H:10:GLY:O	2:H:12:VAL:HG23	2.13	0.47
2:I:20:ILE:HG12	2:I:114:THR:HG21	1.97	0.47
3:L:39:GLN:HE21	3:L:49:LEU:HD21	1.79	0.47
1:C:826:VAL:HG23	1:C:945:LEU:HD23	1.94	0.47
2:I:104:TYR:CD1	3:M:58:PRO:HD3	2.49	0.47
1:A:102:ARG:NH2	1:A:122:ASN:OD1	2.48	0.47
1:A:707:TYR:HB2	1:C:883:THR:CG2	2.44	0.47
1:A:709:ASN:HD22	5:O:1:NAG:H83	1.80	0.47
1:C:231:ILE:HG22	1:C:233:ILE:HG23	1.96	0.47
1:C:1050:MET:HE2	1:C:1052:PHE:CZ	2.50	0.47
2:I:104:TYR:CE1	3:M:57:ALA:HA	2.49	0.47
2:I:104:TYR:HE1	3:M:57:ALA:HA	1.80	0.47
1:B:1103:PHE:HZ	4:e:1:NAG:H62	1.80	0.47
1:C:715:PRO:HA	1:C:1072:GLU:HA	1.96	0.47
1:A:309:GLU:O	1:A:313:TYR:OH	2.25	0.47
1:C:189:LEU:HD12	1:C:210:ILE:HD13	1.96	0.47
1:B:83:VAL:HG11	1:B:237:ARG:NH1	2.29	0.47
1:C:329:PHE:HE2	1:C:528:LYS:HB2	1.79	0.47
1:C:618:THR:OG1	1:C:619:GLU:OE1	2.29	0.47
3:L:88:TYR:O	3:L:103:GLY:HA2	2.15	0.47
1:B:726:ILE:HG13	1:B:1061:VAL:HG22	1.96	0.46
1:C:117:LEU:HB2	1:C:233:ILE:HD11	1.97	0.46
1:C:449:TYR:HB3	2:I:28:SER:HB3	1.97	0.46
3:M:37:TRP:CG	3:M:75:LEU:HD22	2.50	0.46
1:B:83:VAL:HG11	1:B:237:ARG:HH12	1.79	0.46
1:B:733:LYS:NZ	1:B:775:ASP:OD2	2.29	0.46
1:A:41:LYS:NZ	1:B:562:PHE:O	2.29	0.46
1:A:303:LEU:HD22	1:A:308:VAL:HG22	1.96	0.46
1:B:433:VAL:C	1:B:434:ILE:HD13	2.40	0.46
3:M:63:ARG:NH2	3:M:83:GLU:OE1	2.48	0.46
1:A:287:ASP:OD1	1:A:288:ALA:N	2.47	0.46
1:B:33:THR:OG1	1:B:219:GLY:O	2.31	0.46
1:B:215:ASP:OD1	1:B:215:ASP:N	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:529:LYS:HB3	1:B:529:LYS:HE3	1.75	0.46
1:A:328:ARG:HH12	1:A:533:LEU:HD13	1.79	0.46
1:B:199:GLY:HA2	1:B:232:GLY:HA2	1.97	0.46
2:I:47:TRP:CH2	2:I:49:GLY:HA2	2.51	0.46
1:B:377:PHE:CD1	1:B:434:ILE:HD12	2.50	0.46
1:C:277:LEU:HD23	1:C:285:ILE:HD13	1.97	0.46
3:L:85:GLU:OE1	3:L:105:LYS:NZ	2.49	0.46
4:v:2:NAG:H4	4:v:3:BMA:H2	1.68	0.46
1:A:703:ASN:ND2	1:C:787:GLN:OE1	2.49	0.46
1:A:770:ILE:HD11	1:A:1012:LEU:HD23	1.98	0.46
1:B:170:TYR:CZ	1:B:172:SER:HB2	2.51	0.46
1:B:1135:ASN:OD1	1:B:1136:THR:N	2.40	0.46
1:C:986:PRO:N	1:C:987:PRO:HD2	2.31	0.46
4:v:2:NAG:O4	4:v:2:NAG:O7	2.34	0.46
1:B:449:TYR:HB3	2:H:28:SER:CB	2.32	0.46
1:C:332:ILE:HG13	1:C:362:VAL:HG23	1.98	0.46
1:B:290:ASP:O	1:B:297:SER:HB3	2.16	0.45
1:B:339:GLY:O	1:B:343:ASN:HB2	2.17	0.45
1:C:102:ARG:HG3	1:C:102:ARG:HH11	1.81	0.45
2:H:86:GLN:NE2	2:H:89:ASP:OD2	2.49	0.45
1:A:555:SER:HB3	1:A:586:ASP:CG	2.41	0.45
2:I:36:TRP:HE1	2:I:78:VAL:HG12	1.81	0.45
3:M:17:THR:HA	3:M:78:THR:HA	1.99	0.45
1:A:29:THR:HG22	1:A:30:ASN:N	2.31	0.45
1:B:95:THR:HG22	1:B:189:LEU:HD13	1.97	0.45
1:B:380:TYR:HD2	1:B:429:PHE:CD2	2.34	0.45
2:H:12:VAL:HG11	2:H:85:LEU:HD22	1.99	0.45
3:L:23:ARG:HA	3:L:72:LYS:HG2	1.97	0.45
5:Y:1:NAG:H82	5:Y:2:NAG:H83	1.97	0.45
1:B:65:PHE:O	1:B:264:ALA:HB1	2.17	0.45
1:A:329:PHE:HB3	1:A:330:PRO:HD2	1.98	0.45
1:B:319:ARG:HG2	1:B:319:ARG:HH11	1.81	0.45
1:B:449:TYR:CG	2:H:28:SER:HB3	2.51	0.45
1:B:484:GLU:CD	2:H:52:TRP:HB3	2.42	0.45
1:C:309:GLU:O	1:C:313:TYR:OH	2.20	0.45
1:B:201:PHE:HB3	1:B:229:LEU:HB2	1.98	0.45
1:B:418:ILE:HA	1:B:422:ASN:OD1	2.16	0.45
1:C:418:ILE:HD12	1:C:422:ASN:OD1	2.17	0.45
2:H:92:ARG:HG2	2:H:115:SER:HA	1.97	0.45
3:L:38:VAL:HG22	3:L:89:PHE:HB2	1.97	0.45
1:C:65:PHE:CE2	1:C:84:LEU:HD21	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:426:PRO:HB3	1:C:463:PRO:HB3	1.98	0.45
1:C:1028:LYS:NZ	1:C:1042:PHE:O	2.45	0.45
2:I:4:LEU:HD13	2:I:24:VAL:HG12	1.97	0.45
2:I:98:LYS:HG2	2:I:107:MET:SD	2.57	0.45
1:A:743:CYS:HB3	1:A:749:CYS:HB3	1.78	0.45
2:H:19:SER:HB2	2:H:81:LYS:HD2	1.98	0.45
1:A:1098:ASN:OD1	1:A:1100:THR:N	2.39	0.44
3:M:23:ARG:HB3	3:M:72:LYS:HZ3	1.81	0.44
1:A:97:LYS:HZ1	1:A:188:ASN:N	2.15	0.44
1:B:453:TYR:HE1	1:B:495:TYR:HD1	1.64	0.44
1:C:32:PHE:CG	1:C:218:GLN:HG2	2.52	0.44
1:C:358:ILE:HB	1:C:395:VAL:CG2	2.47	0.44
1:C:977:LEU:HD11	1:C:993:ILE:HD12	1.99	0.44
2:H:86:GLN:NE2	2:H:88:ASP:HB2	2.31	0.44
1:A:227:VAL:HG12	1:A:229:LEU:HD22	2.00	0.44
1:C:103:GLY:HA3	1:C:241:LEU:HD13	1.99	0.44
3:M:3:VAL:HB	3:M:25:SER:HB2	1.99	0.44
1:A:405:ASP:CB	3:L:69:ILE:O	2.65	0.44
1:B:376:THR:HG22	1:B:435:ALA:HB3	2.00	0.44
1:C:197:ILE:O	1:C:200:TYR:HB2	2.16	0.44
1:A:65:PHE:CZ	1:A:84:LEU:HD21	2.52	0.44
1:B:405:ASP:N	1:B:504:GLY:O	2.49	0.44
1:C:559:PHE:HB2	1:C:563:GLN:OE1	2.17	0.44
2:I:29:LEU:O	2:I:53:THR:OG1	2.31	0.44
1:A:101:ILE:HD13	1:A:101:ILE:HA	1.91	0.44
1:C:758:SER:O	1:C:762:GLN:HG2	2.18	0.44
2:I:35:SER:O	2:I:96:ALA:N	2.50	0.44
1:B:366:SER:HB2	1:B:388:ASN:ND2	2.32	0.44
1:C:821:LEU:O	1:C:825:LYS:HG2	2.18	0.44
2:H:45:LEU:HD21	3:L:100:PHE:HB3	1.98	0.44
2:I:34:ILE:HG21	2:I:78:VAL:HG21	1.99	0.44
3:M:83:GLU:OE2	3:M:83:GLU:N	2.51	0.44
1:A:46:SER:HA	1:A:279:TYR:O	2.17	0.44
1:A:375:SER:N	1:A:435:ALA:O	2.51	0.44
1:B:605:SER:OG	1:B:606:ASN:N	2.50	0.44
1:B:722:VAL:HG22	1:B:1065:VAL:HG22	2.00	0.44
1:C:31:SER:HA	1:C:216:LEU:HD11	1.99	0.44
2:H:98:LYS:HZ1	2:H:100:TYR:HD2	1.64	0.44
1:B:518:LEU:HD12	1:B:518:LEU:HA	1.86	0.44
1:C:433:VAL:HG12	1:C:512:VAL:HG22	1.99	0.44
1:C:1029:MET:HE2	1:C:1029:MET:HB2	1.84	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:39:GLN:NE2	2:H:40:PRO:O	2.44	0.44
1:A:58:PHE:HB3	1:A:59:PHE:HD1	1.83	0.43
1:A:887:THR:HG21	1:A:894:LEU:HD12	1.99	0.43
1:B:811:LYS:HD3	1:B:813:SER:N	2.29	0.43
3:M:2:ALA:O	3:M:99:VAL:HG21	2.17	0.43
3:M:10:LEU:HD11	3:M:20:LEU:HB3	2.00	0.43
1:A:326:ILE:HD12	1:A:532:ASN:O	2.17	0.43
1:A:858:LEU:HD13	1:A:959:LEU:HD22	2.00	0.43
1:C:452:LEU:HG	1:C:494:SER:HB2	1.99	0.43
1:A:97:LYS:HA	1:A:97:LYS:HE2	2.01	0.43
1:C:404:GLY:HA2	1:C:508:TYR:CG	2.54	0.43
1:C:731:MET:HE2	1:C:1015:ALA:HA	2.00	0.43
1:A:718:PHE:HE1	1:A:923:ILE:HG12	1.83	0.43
1:A:737:ASP:OD1	1:A:737:ASP:N	2.50	0.43
1:B:409:GLN:HA	1:B:414:GLN:HG2	2.00	0.43
1:C:34:ARG:NH1	1:C:217:PRO:O	2.51	0.43
1:B:29:THR:HG22	1:B:30:ASN:N	2.27	0.43
1:C:725:GLU:OE2	1:C:1028:LYS:NZ	2.48	0.43
2:H:37:VAL:HG23	2:H:94:TYR:HB2	2.00	0.43
1:B:569:ILE:HD12	1:B:569:ILE:H	1.84	0.43
1:C:494:SER:OG	1:C:495:TYR:N	2.51	0.43
2:I:91:ALA:O	2:I:116:VAL:HB	2.18	0.43
1:A:97:LYS:HG2	1:A:186:PHE:CD1	2.53	0.43
1:B:117:LEU:CD2	1:B:233:ILE:HG21	2.48	0.43
1:B:537:LYS:N	1:B:551:VAL:HG23	2.33	0.43
1:C:329:PHE:CE2	1:C:528:LYS:HB2	2.54	0.43
1:C:417:LYS:HG2	1:C:455:LEU:HD12	2.01	0.43
1:C:443:SER:OG	1:C:497:PHE:O	2.22	0.43
1:A:1050:MET:HG2	1:A:1065:VAL:HB	2.00	0.43
1:B:33:THR:HB	1:B:220:PHE:HD1	1.84	0.43
1:B:354:ASN:OD1	1:B:399:SER:HB3	2.19	0.43
1:B:356:LYS:HB2	1:B:356:LYS:HE3	1.73	0.43
1:C:494:SER:HB2	2:I:30:ILE:CG2	2.49	0.43
1:C:754:LEU:HD12	1:C:754:LEU:HA	1.83	0.43
1:A:984:LEU:HD13	1:A:988:GLU:OE1	2.19	0.43
1:C:190:ARG:HG2	1:C:192:PHE:CE1	2.54	0.43
1:C:598:ILE:HB	1:C:609:ALA:HB3	2.00	0.43
1:B:369:TYR:O	1:B:371:SER:OG	2.32	0.43
1:B:716:THR:HG22	1:B:1110:TYR:HB3	1.99	0.43
1:C:34:ARG:NH1	1:C:34:ARG:HB2	2.34	0.43
1:C:201:PHE:HE2	1:C:203:ILE:HD11	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:20:ILE:CG2	2:I:80:LEU:HB3	2.49	0.43
3:L:37:TRP:HD1	3:L:50:ILE:HB	1.83	0.43
1:B:1086:LYS:HB2	1:B:1086:LYS:HE2	1.69	0.42
1:C:976:VAL:HB	1:C:979:ASP:HB2	2.01	0.42
2:H:67:LEU:HD22	2:H:82:MET:SD	2.59	0.42
2:I:22:CYS:N	2:I:78:VAL:O	2.35	0.42
3:L:81:GLN:OE1	3:L:82:THR:OG1	2.36	0.42
3:M:85:GLU:CD	3:M:108:VAL:HG22	2.44	0.42
1:A:40:ASP:OD1	1:A:40:ASP:N	2.49	0.42
1:A:1114:ILE:HD12	1:A:1114:ILE:H	1.84	0.42
1:C:354:ASN:O	1:C:398:ASP:HA	2.18	0.42
1:C:580:GLN:O	5:l:2:NAG:O6	2.27	0.42
1:C:1086:LYS:HB3	1:C:1122:VAL:HG13	2.02	0.42
1:A:325:SER:O	1:A:326:ILE:HD13	2.20	0.42
1:C:393:THR:HG21	1:C:518:LEU:HB3	2.00	0.42
3:L:41:LYS:HD3	3:L:42:PRO:HD2	2.00	0.42
1:A:981:LEU:HD23	1:A:981:LEU:HA	1.81	0.42
1:B:584:ILE:HG13	1:B:584:ILE:O	2.19	0.42
1:C:30:ASN:HB3	1:C:32:PHE:CZ	2.55	0.42
2:I:32:TYR:HD2	2:I:99:ASP:HA	1.84	0.42
1:B:200:TYR:HD1	1:B:228:ASP:OD1	2.03	0.42
1:C:449:TYR:OH	2:I:26:GLY:C	2.62	0.42
2:I:86:GLN:NE2	2:I:89:ASP:OD2	2.52	0.42
1:B:411:ALA:HB3	1:B:414:GLN:HB2	2.02	0.42
1:B:796:ASP:OD1	1:B:796:ASP:N	2.48	0.42
1:B:1049:LEU:O	1:B:1050:MET:HB3	2.19	0.42
1:C:105:ILE:HG12	1:C:241:LEU:HD11	2.00	0.42
1:C:353:TRP:HZ3	1:C:355:ARG:HD2	1.84	0.42
3:M:27:GLY:O	3:M:72:LYS:HE2	2.20	0.42
1:A:557:LYS:HB2	1:A:584:ILE:CD1	2.48	0.42
2:I:4:LEU:C	2:I:5:LYS:HD3	2.45	0.42
3:L:29:VAL:HG22	3:L:72:LYS:HA	2.01	0.42
1:A:567:ARG:HH21	1:C:42:VAL:HG21	1.85	0.42
1:B:393:THR:O	1:B:523:THR:HG22	2.19	0.42
5:k:1:NAG:H5	5:k:2:NAG:C7	2.49	0.42
1:B:443:SER:HB2	1:B:507:PRO:HG3	2.01	0.42
1:B:449:TYR:CD1	1:B:496:GLY:HA2	2.54	0.42
2:H:12:VAL:HG12	2:H:13:ALA:O	2.19	0.42
1:B:537:LYS:HB3	1:B:537:LYS:HE2	1.73	0.42
1:B:869:MET:HG2	1:C:699:LEU:HD11	2.02	0.42
1:C:83:VAL:HG22	1:C:239:GLN:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:86:GLN:HG3	2:H:89:ASP:OD1	2.20	0.42
1:A:462:LYS:HA	1:A:463:PRO:HD3	1.93	0.41
1:A:905:ARG:HD2	1:A:1049:LEU:O	2.20	0.41
1:B:903:ALA:HB1	1:B:913:GLN:HB2	2.02	0.41
1:B:115:GLN:H	1:B:115:GLN:CD	2.28	0.41
1:B:503:VAL:HA	1:B:506:GLN:HG2	2.02	0.41
1:A:130:VAL:HG21	1:A:233:ILE:HG21	2.02	0.41
3:M:39:GLN:HE22	3:M:41:LYS:HD2	1.85	0.41
1:B:101:ILE:HD11	1:B:240:THR:OG1	2.19	0.41
1:B:227:VAL:HG12	1:B:229:LEU:HD12	2.01	0.41
1:B:337:PRO:HB2	1:B:340:GLU:CG	2.51	0.41
1:C:34:ARG:HB2	1:C:34:ARG:HH11	1.85	0.41
1:C:474:GLN:OE1	1:C:480:CYS:N	2.54	0.41
1:C:1012:LEU:HD23	1:C:1012:LEU:HA	1.89	0.41
3:M:4:VAL:HA	3:M:23:ARG:O	2.21	0.41
1:C:513:LEU:HD23	1:C:513:LEU:HA	1.96	0.41
2:H:13:ALA:HB3	2:H:16:GLN:HE22	1.85	0.41
2:I:22:CYS:HB3	2:I:78:VAL:HB	2.02	0.41
1:B:27:ALA:HB3	1:B:64:TRP:CE3	2.50	0.41
3:M:14:PRO:HG3	3:M:81:GLN:CD	2.46	0.41
1:B:106:PHE:O	1:B:116:SER:HB2	2.20	0.41
1:C:474:GLN:HE22	1:C:479:PRO:HA	1.85	0.41
1:C:560:LEU:HB3	1:C:561:PRO:HD2	2.03	0.41
1:A:328:ARG:HH21	1:A:580:GLN:HB2	1.85	0.41
1:A:765:ARG:CZ	1:B:957:GLN:HE21	2.32	0.41
1:A:1031:GLU:OE2	1:B:1039:ARG:NH2	2.54	0.41
1:B:43:PHE:HE2	1:C:557:LYS:HG2	1.85	0.41
1:B:229:LEU:HB3	1:B:231:ILE:HG12	2.02	0.41
1:B:328:ARG:NH2	1:B:580:GLN:HB2	2.36	0.41
1:B:375:SER:N	1:B:435:ALA:O	2.53	0.41
1:B:388:ASN:O	1:B:526:GLY:HA3	2.20	0.41
1:C:398:ASP:OD2	1:C:423:TYR:OH	2.35	0.41
1:C:420:ASP:O	1:C:461:LEU:HB2	2.20	0.41
1:C:560:LEU:O	1:C:563:GLN:HB2	2.21	0.41
1:C:878:LEU:HD21	1:C:1052:PHE:HB3	2.02	0.41
2:H:24:VAL:HB	2:H:27:PHE:CZ	2.56	0.41
2:I:37:VAL:HG12	2:I:47:TRP:HA	2.02	0.41
2:I:38:ARG:HB3	2:I:48:LEU:HD21	2.02	0.41
3:L:35:ALA:HA	3:L:91:ALA:O	2.21	0.41
1:A:240:THR:HG21	1:A:265:TYR:CZ	2.56	0.41
1:B:731:MET:N	1:B:774:GLN:OE1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:312:ILE:HD13	1:C:598:ILE:HG13	2.03	0.41
1:C:352:ALA:HB1	1:C:466:ARG:HH21	1.85	0.41
2:H:66:ARG:HG2	2:H:83:ASN:ND2	2.30	0.41
3:L:29:VAL:O	3:L:68:LEU:HD11	2.20	0.40
1:A:534:VAL:HG23	1:A:539:VAL:HG11	2.03	0.40
1:B:403:ARG:HG3	1:B:505:TYR:HA	2.03	0.40
1:B:501:ASN:OD1	1:B:502:GLY:N	2.48	0.40
3:M:69:ILE:H	3:M:69:ILE:HD12	1.86	0.40
1:A:118:LEU:HD21	1:A:120:VAL:HB	2.04	0.40
1:A:388:ASN:O	1:A:526:GLY:HA3	2.21	0.40
1:C:897:PRO:HD2	1:C:900:MET:HE3	2.04	0.40
2:I:38:ARG:HD2	2:I:91:ALA:HB3	2.02	0.40
1:A:749:CYS:SG	1:A:997:ILE:HD11	2.61	0.40
1:B:736:VAL:HG22	1:B:858:LEU:HD23	2.03	0.40
1:B:1135:ASN:CG	1:B:1136:THR:H	2.27	0.40
3:L:52:GLY:C	3:L:54:ASN:H	2.29	0.40
1:A:102:ARG:NH2	1:A:121:ASN:O	2.43	0.40
1:B:334:ASN:OD1	1:B:334:ASN:N	2.54	0.40
1:B:341:VAL:HG13	1:B:342:PHE:CD1	2.49	0.40
1:B:904:TYR:HE1	1:C:1107:ARG:HD3	1.85	0.40
1:B:1106:GLN:HE21	1:B:1109:PHE:HB3	1.85	0.40
1:C:736:VAL:HG13	1:C:858:LEU:HD23	2.04	0.40
2:H:87:THR:O	2:H:90:THR:HG22	2.22	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	924/1256 (74%)	885 (96%)	39 (4%)	0	100	100
1	B	978/1256 (78%)	931 (95%)	47 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	975/1256 (78%)	929 (95%)	46 (5%)	0	100	100
2	H	117/119 (98%)	115 (98%)	2 (2%)	0	100	100
2	I	117/119 (98%)	116 (99%)	1 (1%)	0	100	100
3	L	107/109 (98%)	103 (96%)	4 (4%)	0	100	100
3	M	107/109 (98%)	103 (96%)	4 (4%)	0	100	100
All	All	3325/4224 (79%)	3182 (96%)	143 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	684/1093 (63%)	683 (100%)	1 (0%)	88	91
1	B	838/1093 (77%)	838 (100%)	0	100	100
1	C	831/1093 (76%)	827 (100%)	4 (0%)	81	85
2	H	101/101 (100%)	101 (100%)	0	100	100
2	I	101/101 (100%)	101 (100%)	0	100	100
3	L	86/86 (100%)	86 (100%)	0	100	100
3	M	86/86 (100%)	86 (100%)	0	100	100
All	All	2727/3653 (75%)	2722 (100%)	5 (0%)	85	89

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1029	MET
1	C	429	PHE
1	C	514	SER
1	C	1028	LYS
1	C	1029	MET

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

Mol	Chain	Res	Type
1	A	196	ASN
1	A	314	GLN
1	A	317	ASN
1	A	343	ASN
1	A	540	ASN
1	A	690	GLN
1	A	703	ASN
1	A	804	GLN
1	A	926	GLN
1	A	1002	GLN
1	B	439	ASN
1	B	563	GLN
1	B	607	GLN
1	B	804	GLN
1	B	957	GLN
1	B	1058	HIS
1	C	239	GLN
1	C	394	ASN
1	C	450	ASN
1	C	804	GLN
1	C	928	ASN
1	C	960	ASN
1	C	1083	HIS
2	H	16	GLN
2	I	16	GLN
3	L	55	ASN
3	M	36	ASN
3	M	55	ASN
3	M	81	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 ⓘ

102 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
4	NAG	D	1	1,4	14,14,15	0.65	1 (7%)	17,19,21	0.90	1 (5%)
4	NAG	D	2	4	14,14,15	0.79	1 (7%)	17,19,21	1.43	1 (5%)
4	BMA	D	3	4	11,11,12	0.91	0	15,15,17	0.91	0
4	NAG	E	1	1,4	14,14,15	0.38	0	17,19,21	0.35	0
4	NAG	E	2	4	14,14,15	0.48	0	17,19,21	0.44	0
4	BMA	E	3	4	11,11,12	0.90	0	15,15,17	0.91	1 (6%)
5	NAG	F	1	1,5	14,14,15	0.17	0	17,19,21	0.48	0
5	NAG	F	2	5	14,14,15	0.62	1 (7%)	17,19,21	0.76	0
5	NAG	G	1	1,5	14,14,15	0.31	0	17,19,21	0.35	0
5	NAG	G	2	5	14,14,15	0.36	0	17,19,21	0.46	0
6	NAG	J	1	6,1	14,14,15	0.85	1 (7%)	17,19,21	0.83	1 (5%)
6	FUC	J	2	6	10,10,11	0.71	0	14,14,16	0.81	0
5	NAG	K	1	1,5	14,14,15	0.94	2 (14%)	17,19,21	1.11	1 (5%)
5	NAG	K	2	5	14,14,15	0.94	2 (14%)	17,19,21	0.52	0
5	NAG	N	1	1,5	14,14,15	0.93	1 (7%)	17,19,21	1.18	1 (5%)
5	NAG	N	2	5	14,14,15	0.95	2 (14%)	17,19,21	0.52	0
5	NAG	O	1	1,5	14,14,15	0.24	0	17,19,21	0.39	0
5	NAG	O	2	5	14,14,15	0.28	0	17,19,21	0.41	0
7	NAG	P	1	1,7	14,14,15	0.30	0	17,19,21	0.50	0
7	NAG	P	2	7	14,14,15	0.60	0	17,19,21	1.82	3 (17%)
7	BMA	P	3	7	11,11,12	0.57	0	15,15,17	0.67	0
7	MAN	P	4	7	11,11,12	0.61	0	15,15,17	0.99	2 (13%)
5	NAG	Q	1	1,5	14,14,15	0.52	0	17,19,21	0.42	0
5	NAG	Q	2	5	14,14,15	0.27	0	17,19,21	0.36	0
5	NAG	R	1	1,5	14,14,15	0.24	0	17,19,21	0.55	0
5	NAG	R	2	5	14,14,15	0.26	0	17,19,21	0.39	0
4	NAG	S	1	1,4	14,14,15	1.26	1 (7%)	17,19,21	1.15	1 (5%)
4	NAG	S	2	4	14,14,15	0.22	0	17,19,21	0.70	1 (5%)
4	BMA	S	3	4	11,11,12	0.98	1 (9%)	15,15,17	1.26	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	T	1	1,4	14,14,15	0.21	0	17,19,21	0.48	0
4	NAG	T	2	4	14,14,15	0.20	0	17,19,21	0.51	0
4	BMA	T	3	4	11,11,12	0.59	0	15,15,17	0.71	0
7	NAG	U	1	1,7	14,14,15	0.37	0	17,19,21	0.48	0
7	NAG	U	2	7	14,14,15	0.62	1 (7%)	17,19,21	0.99	2 (11%)
7	BMA	U	3	7	11,11,12	0.69	0	15,15,17	0.81	0
7	MAN	U	4	7	11,11,12	0.57	0	15,15,17	0.99	2 (13%)
4	NAG	V	1	1,4	14,14,15	0.39	0	17,19,21	0.37	0
4	NAG	V	2	4	14,14,15	0.66	1 (7%)	17,19,21	0.60	0
4	BMA	V	3	4	11,11,12	1.06	1 (9%)	15,15,17	1.10	1 (6%)
4	NAG	W	1	1,4	14,14,15	0.40	0	17,19,21	0.37	0
4	NAG	W	2	4	14,14,15	0.49	0	17,19,21	0.55	0
4	BMA	W	3	4	11,11,12	0.55	0	15,15,17	0.71	0
5	NAG	X	1	1,5	14,14,15	0.37	0	17,19,21	0.47	0
5	NAG	X	2	5	14,14,15	0.53	0	17,19,21	1.06	2 (11%)
5	NAG	Y	1	1,5	14,14,15	0.29	0	17,19,21	1.31	1 (5%)
5	NAG	Y	2	5	14,14,15	0.33	0	17,19,21	0.53	0
5	NAG	Z	1	1,5	14,14,15	0.28	0	17,19,21	0.51	0
5	NAG	Z	2	5	14,14,15	0.45	0	17,19,21	0.60	0
4	NAG	a	1	1,4	14,14,15	0.41	0	17,19,21	0.61	0
4	NAG	a	2	4	14,14,15	0.17	0	17,19,21	0.42	0
4	BMA	a	3	4	11,11,12	0.63	0	15,15,17	0.69	0
6	NAG	b	1	6,1	14,14,15	0.71	1 (7%)	17,19,21	0.50	0
6	FUC	b	2	6	10,10,11	0.64	0	14,14,16	0.89	0
5	NAG	c	1	1,5	14,14,15	0.96	1 (7%)	17,19,21	1.16	1 (5%)
5	NAG	c	2	5	14,14,15	0.24	0	17,19,21	0.58	0
5	NAG	d	1	1,5	14,14,15	0.22	0	17,19,21	0.42	0
5	NAG	d	2	5	14,14,15	0.18	0	17,19,21	0.45	0
4	NAG	e	1	1,4	14,14,15	0.24	0	17,19,21	0.50	0
4	NAG	e	2	4	14,14,15	0.26	0	17,19,21	0.66	0
4	BMA	e	3	4	11,11,12	1.02	1 (9%)	15,15,17	1.22	1 (6%)
5	NAG	f	1	1,5	14,14,15	0.65	0	17,19,21	0.49	0
5	NAG	f	2	5	14,14,15	0.26	0	17,19,21	0.36	0
5	NAG	g	1	1,5	14,14,15	0.26	0	17,19,21	0.49	0
5	NAG	g	2	5	14,14,15	0.20	0	17,19,21	0.39	0
4	NAG	h	1	1,4	14,14,15	0.20	0	17,19,21	0.47	0
4	NAG	h	2	4	14,14,15	0.21	0	17,19,21	0.51	0
4	BMA	h	3	4	11,11,12	0.66	0	15,15,17	0.69	0
4	NAG	i	1	1,4	14,14,15	1.08	2 (14%)	17,19,21	1.70	3 (17%)
4	NAG	i	2	4	14,14,15	0.44	0	17,19,21	0.74	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	BMA	i	3	4	11,11,12	0.99	1 (9%)	15,15,17	1.07	0
4	NAG	j	1	1,4	14,14,15	0.43	0	17,19,21	0.42	0
4	NAG	j	2	4	14,14,15	0.47	0	17,19,21	0.43	0
4	BMA	j	3	4	11,11,12	0.97	0	15,15,17	0.92	1 (6%)
5	NAG	k	1	1,5	14,14,15	0.42	0	17,19,21	1.31	1 (5%)
5	NAG	k	2	5	14,14,15	0.53	0	17,19,21	0.79	0
5	NAG	l	1	1,5	14,14,15	0.36	0	17,19,21	0.45	0
5	NAG	l	2	5	14,14,15	0.43	0	17,19,21	0.42	0
4	NAG	m	1	1,4	14,14,15	0.44	0	17,19,21	0.47	0
4	NAG	m	2	4	14,14,15	1.03	1 (7%)	17,19,21	1.37	1 (5%)
4	BMA	m	3	4	11,11,12	0.62	0	15,15,17	0.70	0
6	NAG	n	1	6,1	14,14,15	0.42	0	17,19,21	0.42	0
6	FUC	n	2	6	10,10,11	0.62	0	14,14,16	0.81	0
5	NAG	o	1	1,5	14,14,15	0.74	1 (7%)	17,19,21	1.20	1 (5%)
5	NAG	o	2	5	14,14,15	0.96	1 (7%)	17,19,21	1.26	1 (5%)
5	NAG	p	1	1,5	14,14,15	0.66	0	17,19,21	0.89	1 (5%)
5	NAG	p	2	5	14,14,15	0.42	0	17,19,21	0.39	0
5	NAG	q	1	1,5	14,14,15	0.28	0	17,19,21	0.34	0
5	NAG	q	2	5	14,14,15	0.22	0	17,19,21	0.44	0
7	NAG	r	1	1,7	14,14,15	0.37	0	17,19,21	0.55	0
7	NAG	r	2	7	14,14,15	0.93	1 (7%)	17,19,21	1.43	1 (5%)
7	BMA	r	3	7	11,11,12	0.68	0	15,15,17	0.87	0
7	MAN	r	4	7	11,11,12	0.82	0	15,15,17	1.26	2 (13%)
5	NAG	s	1	1,5	14,14,15	0.72	0	17,19,21	0.59	0
5	NAG	s	2	5	14,14,15	0.93	1 (7%)	17,19,21	1.33	1 (5%)
5	NAG	t	1	1,5	14,14,15	0.29	0	17,19,21	0.49	0
5	NAG	t	2	5	14,14,15	0.17	0	17,19,21	0.39	0
4	NAG	u	1	1,4	14,14,15	0.88	1 (7%)	17,19,21	1.57	1 (5%)
4	NAG	u	2	4	14,14,15	0.18	0	17,19,21	0.46	0
4	BMA	u	3	4	11,11,12	0.80	0	15,15,17	0.88	0
4	NAG	v	1	1,4	14,14,15	0.36	0	17,19,21	0.42	0
4	NAG	v	2	4	14,14,15	0.74	1 (7%)	17,19,21	0.88	0
4	BMA	v	3	4	11,11,12	0.58	0	15,15,17	0.70	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	D	1	1,4	-	3/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
4	BMA	D	3	4	-	0/2/19/22	0/1/1/1
4	NAG	E	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	E	2	4	-	4/6/23/26	0/1/1/1
4	BMA	E	3	4	-	1/2/19/22	0/1/1/1
5	NAG	F	1	1,5	-	4/6/23/26	0/1/1/1
5	NAG	F	2	5	-	4/6/23/26	0/1/1/1
5	NAG	G	1	1,5	-	3/6/23/26	0/1/1/1
5	NAG	G	2	5	-	3/6/23/26	0/1/1/1
6	NAG	J	1	6,1	-	4/6/23/26	0/1/1/1
6	FUC	J	2	6	-	-	0/1/1/1
5	NAG	K	1	1,5	-	4/6/23/26	0/1/1/1
5	NAG	K	2	5	-	4/6/23/26	0/1/1/1
5	NAG	N	1	1,5	-	4/6/23/26	0/1/1/1
5	NAG	N	2	5	-	1/6/23/26	0/1/1/1
5	NAG	O	1	1,5	-	4/6/23/26	0/1/1/1
5	NAG	O	2	5	-	2/6/23/26	0/1/1/1
7	NAG	P	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	P	2	7	-	2/6/23/26	0/1/1/1
7	BMA	P	3	7	-	2/2/19/22	0/1/1/1
7	MAN	P	4	7	-	0/2/19/22	0/1/1/1
5	NAG	Q	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	Q	2	5	-	0/6/23/26	0/1/1/1
5	NAG	R	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	R	2	5	-	2/6/23/26	0/1/1/1
4	NAG	S	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	S	2	4	-	2/6/23/26	0/1/1/1
4	BMA	S	3	4	-	0/2/19/22	0/1/1/1
4	NAG	T	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	T	2	4	-	2/6/23/26	0/1/1/1
4	BMA	T	3	4	-	0/2/19/22	0/1/1/1
7	NAG	U	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	U	2	7	-	2/6/23/26	0/1/1/1
7	BMA	U	3	7	-	2/2/19/22	0/1/1/1
7	MAN	U	4	7	-	0/2/19/22	0/1/1/1
4	NAG	V	1	1,4	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	V	2	4	-	4/6/23/26	0/1/1/1
4	BMA	V	3	4	-	0/2/19/22	0/1/1/1
4	NAG	W	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	W	2	4	-	4/6/23/26	0/1/1/1
4	BMA	W	3	4	-	2/2/19/22	0/1/1/1
5	NAG	X	1	1,5	-	4/6/23/26	0/1/1/1
5	NAG	X	2	5	-	4/6/23/26	0/1/1/1
5	NAG	Y	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	Y	2	5	-	4/6/23/26	0/1/1/1
5	NAG	Z	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	Z	2	5	-	1/6/23/26	0/1/1/1
4	NAG	a	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	a	2	4	-	2/6/23/26	0/1/1/1
4	BMA	a	3	4	-	1/2/19/22	0/1/1/1
6	NAG	b	1	6,1	-	2/6/23/26	0/1/1/1
6	FUC	b	2	6	-	-	0/1/1/1
5	NAG	c	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	c	2	5	-	2/6/23/26	0/1/1/1
5	NAG	d	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	d	2	5	-	2/6/23/26	0/1/1/1
4	NAG	e	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	e	2	4	-	0/6/23/26	0/1/1/1
4	BMA	e	3	4	-	0/2/19/22	0/1/1/1
5	NAG	f	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	f	2	5	-	2/6/23/26	0/1/1/1
5	NAG	g	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	g	2	5	-	0/6/23/26	0/1/1/1
4	NAG	h	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	h	2	4	-	2/6/23/26	0/1/1/1
4	BMA	h	3	4	-	0/2/19/22	0/1/1/1
4	NAG	i	1	1,4	-	3/6/23/26	0/1/1/1
4	NAG	i	2	4	-	2/6/23/26	0/1/1/1
4	BMA	i	3	4	-	0/2/19/22	0/1/1/1
4	NAG	j	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	j	2	4	-	4/6/23/26	0/1/1/1
4	BMA	j	3	4	-	2/2/19/22	0/1/1/1
5	NAG	k	1	1,5	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	k	2	5	-	4/6/23/26	0/1/1/1
5	NAG	l	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	l	2	5	-	2/6/23/26	0/1/1/1
4	NAG	m	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	m	2	4	-	4/6/23/26	0/1/1/1
4	BMA	m	3	4	-	2/2/19/22	0/1/1/1
6	NAG	n	1	6,1	-	0/6/23/26	0/1/1/1
6	FUC	n	2	6	-	-	0/1/1/1
5	NAG	o	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	o	2	5	-	3/6/23/26	0/1/1/1
5	NAG	p	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	p	2	5	-	1/6/23/26	0/1/1/1
5	NAG	q	1	1,5	-	4/6/23/26	0/1/1/1
5	NAG	q	2	5	-	2/6/23/26	0/1/1/1
7	NAG	r	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	r	2	7	-	2/6/23/26	0/1/1/1
7	BMA	r	3	7	-	2/2/19/22	0/1/1/1
7	MAN	r	4	7	-	0/2/19/22	1/1/1/1
5	NAG	s	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	s	2	5	-	2/6/23/26	0/1/1/1
5	NAG	t	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	t	2	5	-	2/6/23/26	0/1/1/1
4	NAG	u	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	u	2	4	-	2/6/23/26	0/1/1/1
4	BMA	u	3	4	-	0/2/19/22	0/1/1/1
4	NAG	v	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	v	2	4	-	1/6/23/26	0/1/1/1
4	BMA	v	3	4	-	0/2/19/22	0/1/1/1

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	S	1	NAG	O5-C1	-4.41	1.36	1.43
4	m	2	NAG	O5-C1	3.74	1.50	1.43
5	o	2	NAG	O5-C1	3.37	1.49	1.43
7	r	2	NAG	O5-C1	3.35	1.49	1.43
5	s	2	NAG	O5-C1	3.33	1.49	1.43
5	c	1	NAG	O5-C1	3.32	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	u	1	NAG	O5-C1	3.17	1.49	1.43
6	J	1	NAG	O5-C1	-3.02	1.38	1.43
4	i	1	NAG	C1-C2	2.89	1.56	1.52
4	D	2	NAG	O5-C1	2.80	1.48	1.43
5	N	1	NAG	O5-C1	2.77	1.48	1.43
5	K	2	NAG	O5-C1	2.70	1.48	1.43
4	i	1	NAG	O5-C1	2.68	1.48	1.43
4	e	3	BMA	C1-C2	2.63	1.58	1.52
4	V	3	BMA	C1-C2	2.59	1.58	1.52
5	K	1	NAG	O5-C1	2.58	1.48	1.43
6	b	1	NAG	O5-C1	-2.53	1.39	1.43
5	N	2	NAG	O5-C1	2.50	1.47	1.43
4	v	2	NAG	O5-C1	-2.48	1.39	1.43
5	N	2	NAG	C1-C2	2.44	1.55	1.52
4	i	3	BMA	C1-C2	2.42	1.58	1.52
4	S	3	BMA	C1-C2	2.38	1.57	1.52
5	K	1	NAG	C1-C2	2.27	1.55	1.52
4	V	2	NAG	C1-C2	2.23	1.55	1.52
5	F	2	NAG	O5-C1	-2.17	1.40	1.43
5	K	2	NAG	C1-C2	2.16	1.55	1.52
4	D	1	NAG	O5-C1	-2.09	1.40	1.43
7	U	2	NAG	O5-C1	-2.07	1.40	1.43
5	o	1	NAG	C1-C2	2.00	1.55	1.52

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	P	2	NAG	C1-O5-C5	6.64	121.09	112.19
4	u	1	NAG	C1-O5-C5	6.20	120.49	112.19
4	i	1	NAG	C1-O5-C5	5.76	119.91	112.19
7	r	2	NAG	C1-O5-C5	5.60	119.69	112.19
4	D	2	NAG	C1-O5-C5	5.57	119.66	112.19
4	m	2	NAG	C1-O5-C5	5.33	119.33	112.19
5	s	2	NAG	C1-O5-C5	5.23	119.20	112.19
5	k	1	NAG	C1-O5-C5	5.02	118.91	112.19
5	o	2	NAG	C1-O5-C5	4.77	118.58	112.19
5	Y	1	NAG	C1-O5-C5	4.76	118.57	112.19
5	N	1	NAG	C1-O5-C5	4.51	118.23	112.19
5	o	1	NAG	C1-O5-C5	4.49	118.20	112.19
5	c	1	NAG	C1-O5-C5	4.34	118.01	112.19
5	K	1	NAG	C1-O5-C5	4.05	117.62	112.19
7	r	4	MAN	C1-O5-C5	3.72	117.18	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	p	1	NAG	C1-O5-C5	3.44	116.79	112.19
4	S	3	BMA	C1-O5-C5	3.27	116.57	112.19
4	e	3	BMA	C1-O5-C5	3.19	116.47	112.19
4	V	3	BMA	C1-O5-C5	3.05	116.27	112.19
4	S	1	NAG	C3-C4-C5	2.91	115.51	110.23
5	X	2	NAG	C1-O5-C5	2.84	115.99	112.19
7	U	2	NAG	C1-O5-C5	2.83	115.98	112.19
7	U	4	MAN	C1-O5-C5	2.61	115.69	112.19
7	P	2	NAG	C3-C4-C5	2.53	114.81	110.23
7	P	4	MAN	C1-O5-C5	2.48	115.51	112.19
4	i	2	NAG	C1-O5-C5	2.35	115.33	112.19
4	i	1	NAG	C2-N2-C7	2.34	126.04	122.90
4	D	1	NAG	C2-N2-C7	2.25	125.92	122.90
5	X	2	NAG	C3-C4-C5	2.24	114.30	110.23
7	P	4	MAN	O2-C2-C3	-2.19	105.62	110.15
4	S	2	NAG	C1-O5-C5	2.18	115.11	112.19
4	i	1	NAG	C1-C2-N2	2.18	113.86	110.43
7	U	4	MAN	O2-C2-C3	-2.16	105.67	110.15
7	U	2	NAG	C3-C4-C5	2.15	114.12	110.23
4	j	3	BMA	C2-C3-C4	2.11	114.58	110.86
7	r	4	MAN	O2-C2-C3	-2.07	105.87	110.15
7	P	2	NAG	O5-C5-C4	2.03	115.76	110.83
4	E	3	BMA	C2-C3-C4	2.01	114.39	110.86
6	J	1	NAG	C3-C4-C5	2.00	113.86	110.23

There are no chirality outliers.

All (191) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	1	NAG	C1-C2-N2-C7
4	i	1	NAG	C1-C2-N2-C7
4	v	2	NAG	C1-C2-N2-C7
4	u	2	NAG	O5-C5-C6-O6
5	K	1	NAG	O5-C5-C6-O6
6	b	1	NAG	O5-C5-C6-O6
4	v	1	NAG	O5-C5-C6-O6
5	l	2	NAG	O5-C5-C6-O6
4	V	2	NAG	O5-C5-C6-O6
5	X	1	NAG	O5-C5-C6-O6
7	r	2	NAG	C4-C5-C6-O6
7	P	3	BMA	O5-C5-C6-O6
4	j	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	F	2	NAG	C4-C5-C6-O6
5	Q	1	NAG	C4-C5-C6-O6
4	D	1	NAG	O5-C5-C6-O6
5	X	2	NAG	C4-C5-C6-O6
4	T	1	NAG	O5-C5-C6-O6
4	i	2	NAG	O5-C5-C6-O6
5	F	1	NAG	O5-C5-C6-O6
5	R	2	NAG	O5-C5-C6-O6
5	d	2	NAG	O5-C5-C6-O6
7	P	2	NAG	O5-C5-C6-O6
7	r	2	NAG	O5-C5-C6-O6
4	V	2	NAG	C4-C5-C6-O6
4	W	2	NAG	C4-C5-C6-O6
4	m	1	NAG	C4-C5-C6-O6
5	l	2	NAG	C4-C5-C6-O6
5	s	2	NAG	C4-C5-C6-O6
4	i	1	NAG	O5-C5-C6-O6
5	f	2	NAG	O5-C5-C6-O6
7	r	3	BMA	O5-C5-C6-O6
6	b	1	NAG	C4-C5-C6-O6
5	F	2	NAG	O5-C5-C6-O6
5	c	2	NAG	O5-C5-C6-O6
5	k	2	NAG	O5-C5-C6-O6
5	X	1	NAG	C4-C5-C6-O6
4	h	1	NAG	O5-C5-C6-O6
4	m	3	BMA	O5-C5-C6-O6
6	J	1	NAG	O5-C5-C6-O6
4	i	2	NAG	C4-C5-C6-O6
5	R	2	NAG	C4-C5-C6-O6
7	r	3	BMA	C4-C5-C6-O6
4	V	1	NAG	O5-C5-C6-O6
4	v	1	NAG	C4-C5-C6-O6
5	c	1	NAG	C4-C5-C6-O6
4	j	1	NAG	O5-C5-C6-O6
4	u	2	NAG	C4-C5-C6-O6
5	K	1	NAG	C4-C5-C6-O6
5	O	1	NAG	O5-C5-C6-O6
7	P	2	NAG	C4-C5-C6-O6
5	X	2	NAG	O5-C5-C6-O6
5	k	1	NAG	O5-C5-C6-O6
4	W	3	BMA	C4-C5-C6-O6
5	c	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	D	1	NAG	C4-C5-C6-O6
4	h	1	NAG	C4-C5-C6-O6
5	k	1	NAG	C4-C5-C6-O6
5	g	1	NAG	O5-C5-C6-O6
5	O	1	NAG	C4-C5-C6-O6
4	T	1	NAG	C4-C5-C6-O6
4	m	3	BMA	C4-C5-C6-O6
5	d	2	NAG	C4-C5-C6-O6
5	g	1	NAG	C4-C5-C6-O6
7	P	3	BMA	C4-C5-C6-O6
4	W	3	BMA	O5-C5-C6-O6
5	Q	1	NAG	O5-C5-C6-O6
5	c	1	NAG	O5-C5-C6-O6
5	s	2	NAG	O5-C5-C6-O6
5	F	1	NAG	C4-C5-C6-O6
5	N	1	NAG	O5-C5-C6-O6
4	u	1	NAG	O5-C5-C6-O6
4	D	2	NAG	C8-C7-N2-C2
4	D	2	NAG	O7-C7-N2-C2
4	E	1	NAG	C8-C7-N2-C2
4	E	1	NAG	O7-C7-N2-C2
4	E	2	NAG	C8-C7-N2-C2
4	E	2	NAG	O7-C7-N2-C2
4	T	2	NAG	C8-C7-N2-C2
4	T	2	NAG	O7-C7-N2-C2
4	V	1	NAG	C8-C7-N2-C2
4	V	1	NAG	O7-C7-N2-C2
4	V	2	NAG	C8-C7-N2-C2
4	V	2	NAG	O7-C7-N2-C2
4	W	1	NAG	C8-C7-N2-C2
4	W	1	NAG	O7-C7-N2-C2
4	W	2	NAG	C8-C7-N2-C2
4	W	2	NAG	O7-C7-N2-C2
4	h	2	NAG	C8-C7-N2-C2
4	h	2	NAG	O7-C7-N2-C2
4	j	1	NAG	C8-C7-N2-C2
4	j	1	NAG	O7-C7-N2-C2
4	j	2	NAG	C8-C7-N2-C2
4	j	2	NAG	O7-C7-N2-C2
4	m	1	NAG	C8-C7-N2-C2
4	m	1	NAG	O7-C7-N2-C2
4	m	2	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
4	m	2	NAG	O7-C7-N2-C2
5	F	1	NAG	C8-C7-N2-C2
5	F	1	NAG	O7-C7-N2-C2
5	G	1	NAG	C8-C7-N2-C2
5	G	1	NAG	O7-C7-N2-C2
5	G	2	NAG	C8-C7-N2-C2
5	G	2	NAG	O7-C7-N2-C2
5	K	1	NAG	C8-C7-N2-C2
5	K	1	NAG	O7-C7-N2-C2
5	K	2	NAG	C8-C7-N2-C2
5	K	2	NAG	O7-C7-N2-C2
5	N	1	NAG	C8-C7-N2-C2
5	N	1	NAG	O7-C7-N2-C2
5	O	1	NAG	C8-C7-N2-C2
5	O	1	NAG	O7-C7-N2-C2
5	X	1	NAG	C8-C7-N2-C2
5	X	1	NAG	O7-C7-N2-C2
5	k	1	NAG	C8-C7-N2-C2
5	k	1	NAG	O7-C7-N2-C2
5	o	1	NAG	C8-C7-N2-C2
5	o	1	NAG	O7-C7-N2-C2
5	q	1	NAG	C8-C7-N2-C2
5	q	1	NAG	O7-C7-N2-C2
5	s	1	NAG	C8-C7-N2-C2
5	s	1	NAG	O7-C7-N2-C2
4	S	2	NAG	O5-C5-C6-O6
7	U	2	NAG	O5-C5-C6-O6
7	r	1	NAG	O5-C5-C6-O6
7	U	2	NAG	C4-C5-C6-O6
4	W	2	NAG	O5-C5-C6-O6
4	a	2	NAG	O5-C5-C6-O6
5	Y	2	NAG	C4-C5-C6-O6
5	q	1	NAG	C4-C5-C6-O6
6	J	1	NAG	C4-C5-C6-O6
4	m	1	NAG	O5-C5-C6-O6
4	i	1	NAG	C4-C5-C6-O6
4	S	2	NAG	C4-C5-C6-O6
7	U	3	BMA	O5-C5-C6-O6
5	Z	1	NAG	O5-C5-C6-O6
5	Y	2	NAG	O5-C5-C6-O6
5	q	1	NAG	O5-C5-C6-O6
4	E	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	V	1	NAG	C4-C5-C6-O6
7	U	1	NAG	O5-C5-C6-O6
5	f	2	NAG	C4-C5-C6-O6
5	l	1	NAG	O5-C5-C6-O6
5	k	2	NAG	C4-C5-C6-O6
5	O	2	NAG	O5-C5-C6-O6
5	K	2	NAG	C4-C5-C6-O6
5	N	1	NAG	C4-C5-C6-O6
7	U	3	BMA	C4-C5-C6-O6
5	K	2	NAG	O5-C5-C6-O6
5	O	2	NAG	C4-C5-C6-O6
5	t	2	NAG	C4-C5-C6-O6
4	m	2	NAG	O5-C5-C6-O6
5	q	2	NAG	C4-C5-C6-O6
5	o	2	NAG	O5-C5-C6-O6
5	t	2	NAG	O5-C5-C6-O6
4	m	2	NAG	C4-C5-C6-O6
7	r	1	NAG	C4-C5-C6-O6
5	G	1	NAG	O5-C5-C6-O6
4	a	3	BMA	O5-C5-C6-O6
5	N	2	NAG	O5-C5-C6-O6
5	Z	2	NAG	O5-C5-C6-O6
4	E	3	BMA	O5-C5-C6-O6
5	q	2	NAG	O5-C5-C6-O6
5	G	2	NAG	O5-C5-C6-O6
5	p	2	NAG	O5-C5-C6-O6
5	F	2	NAG	C1-C2-N2-C7
5	k	2	NAG	C1-C2-N2-C7
5	o	2	NAG	C1-C2-N2-C7
6	J	1	NAG	C1-C2-N2-C7
4	a	2	NAG	C4-C5-C6-O6
5	p	1	NAG	C4-C5-C6-O6
4	E	2	NAG	C4-C5-C6-O6
4	a	1	NAG	C3-C2-N2-C7
5	X	2	NAG	C3-C2-N2-C7
5	Y	2	NAG	C3-C2-N2-C7
6	J	1	NAG	C3-C2-N2-C7
4	j	2	NAG	C4-C5-C6-O6
4	j	2	NAG	O5-C5-C6-O6
5	p	1	NAG	O5-C5-C6-O6
4	j	3	BMA	C4-C5-C6-O6
4	a	1	NAG	C1-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
5	X	2	NAG	C1-C2-N2-C7
5	Y	2	NAG	C1-C2-N2-C7
7	U	1	NAG	C4-C5-C6-O6
5	F	2	NAG	C3-C2-N2-C7
5	k	2	NAG	C3-C2-N2-C7
5	o	2	NAG	C3-C2-N2-C7
5	t	1	NAG	C4-C5-C6-O6
4	j	3	BMA	O5-C5-C6-O6
5	t	1	NAG	O5-C5-C6-O6
4	u	1	NAG	C4-C5-C6-O6

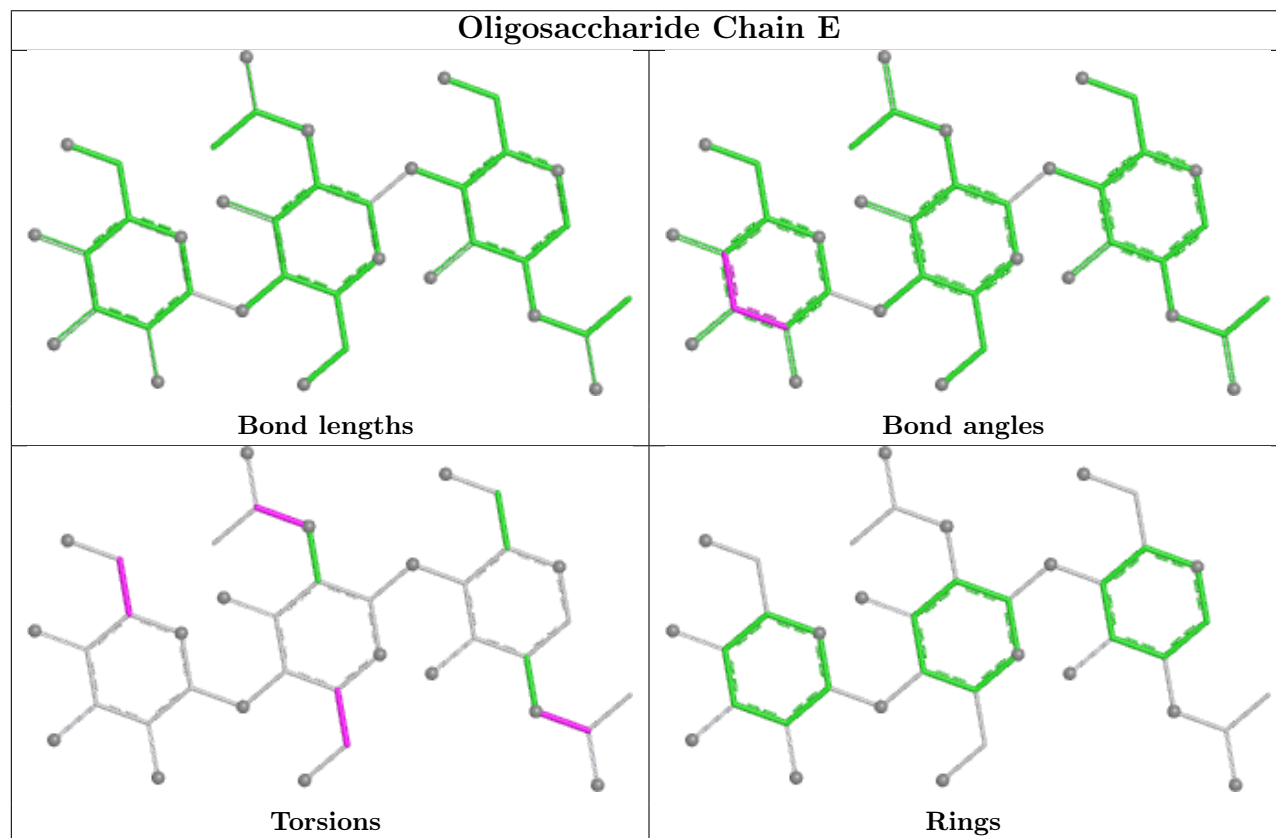
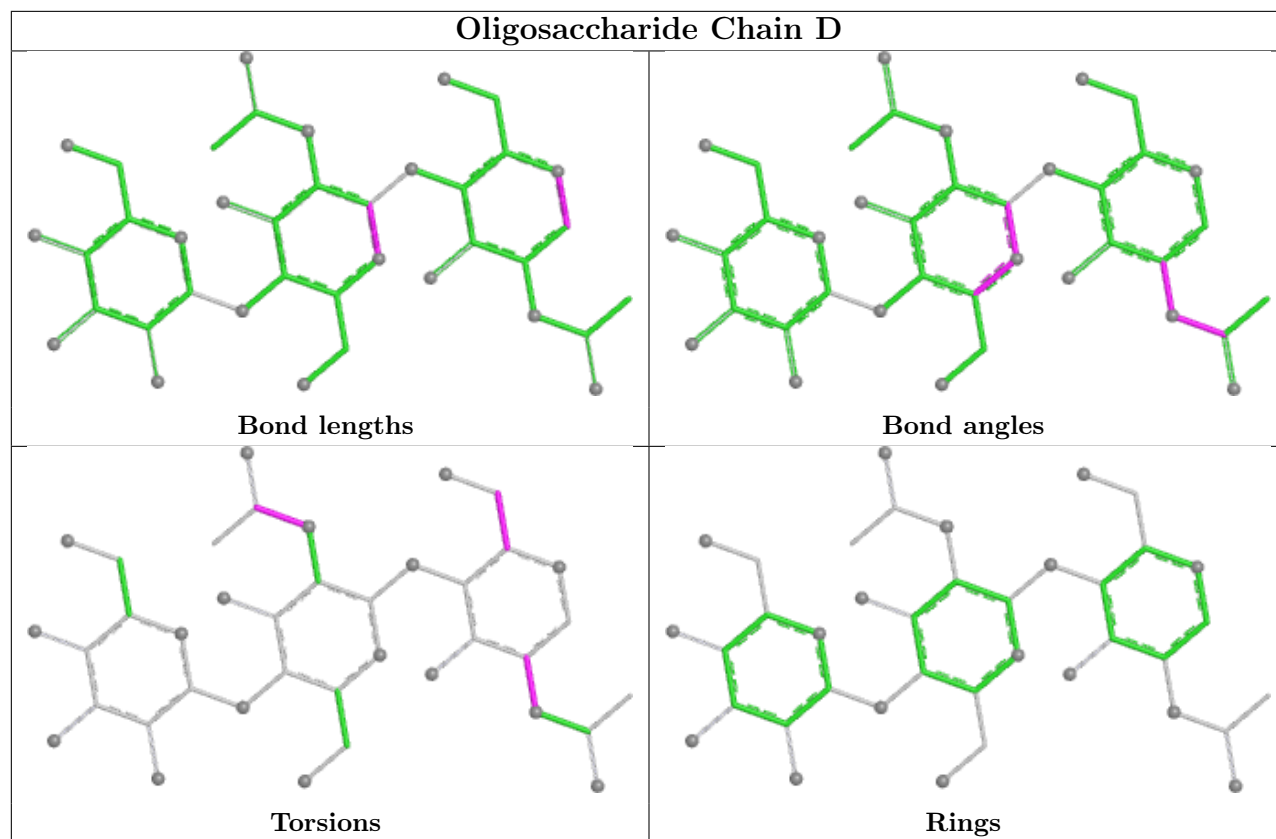
All (1) ring outliers are listed below:

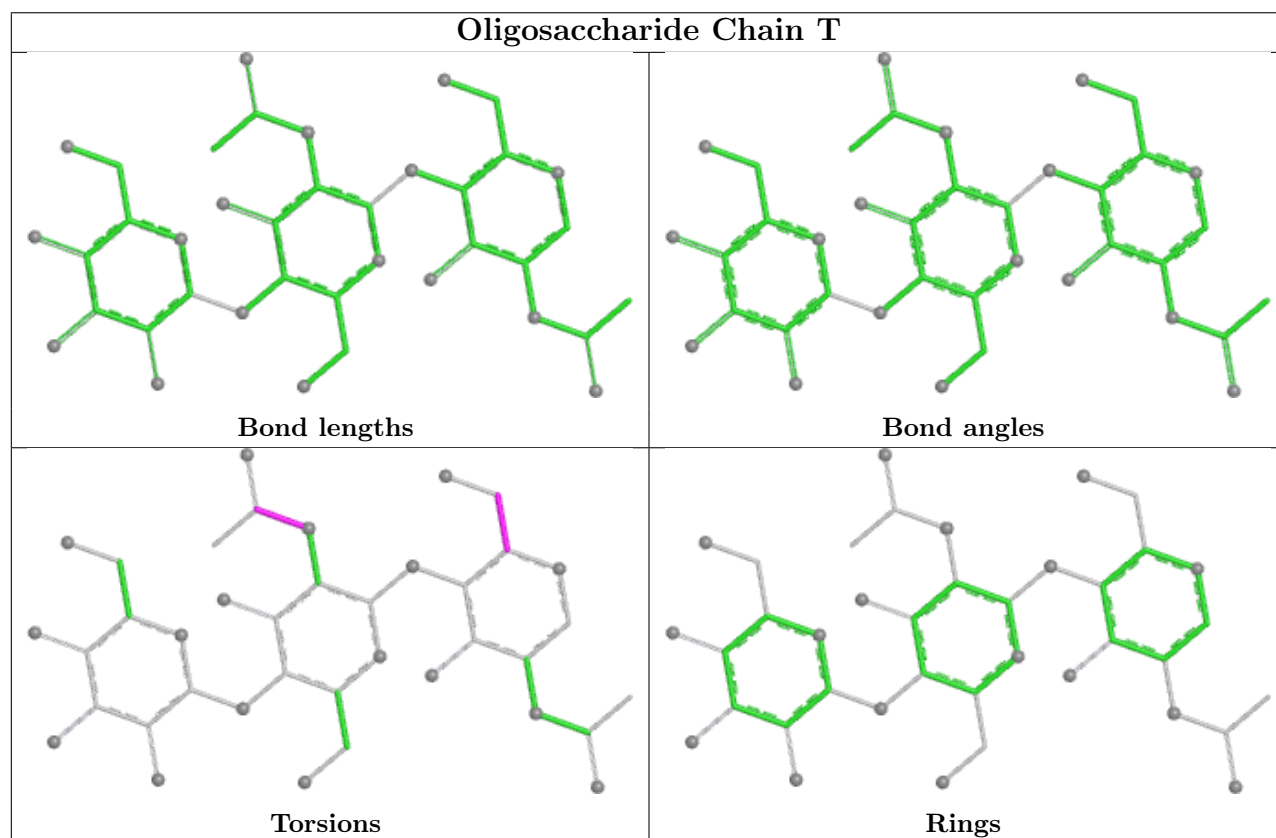
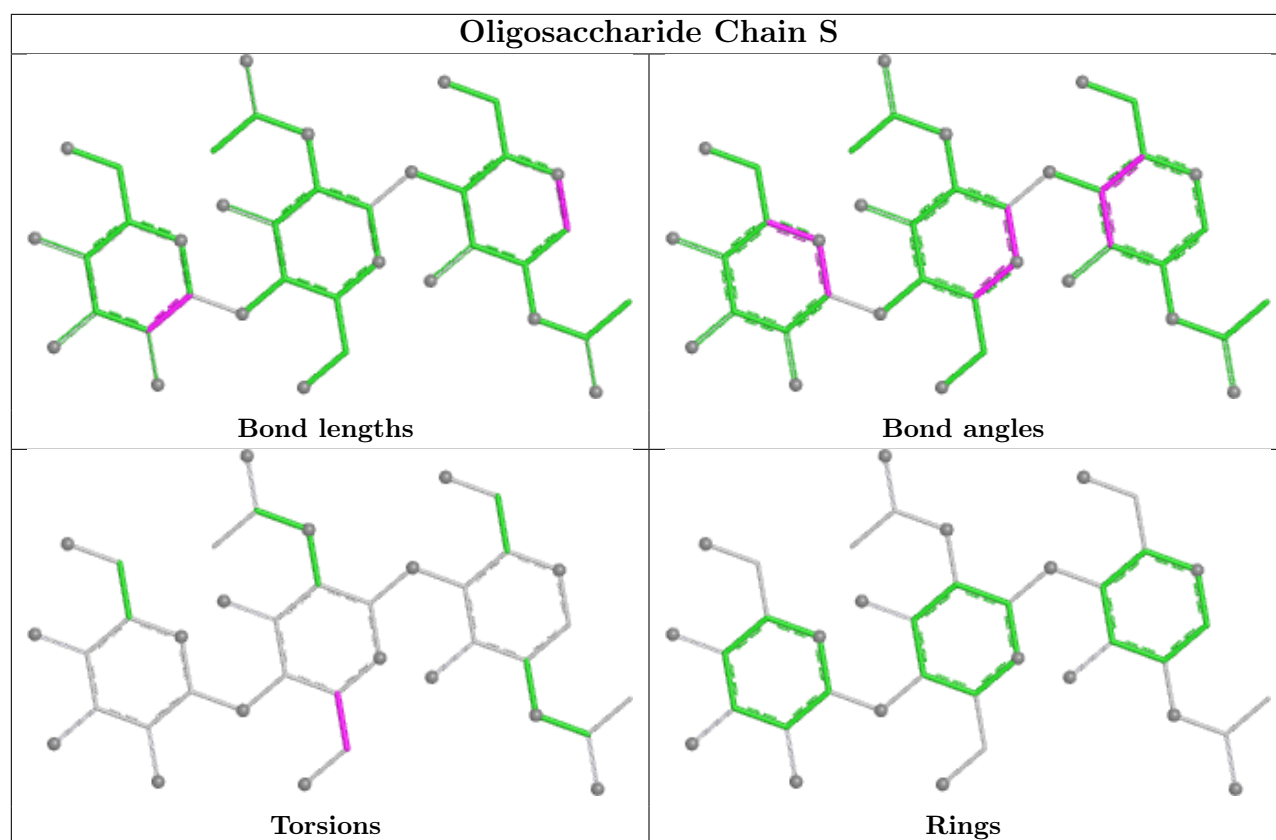
Mol	Chain	Res	Type	Atoms
7	r	4	MAN	C1-C2-C3-C4-C5-O5

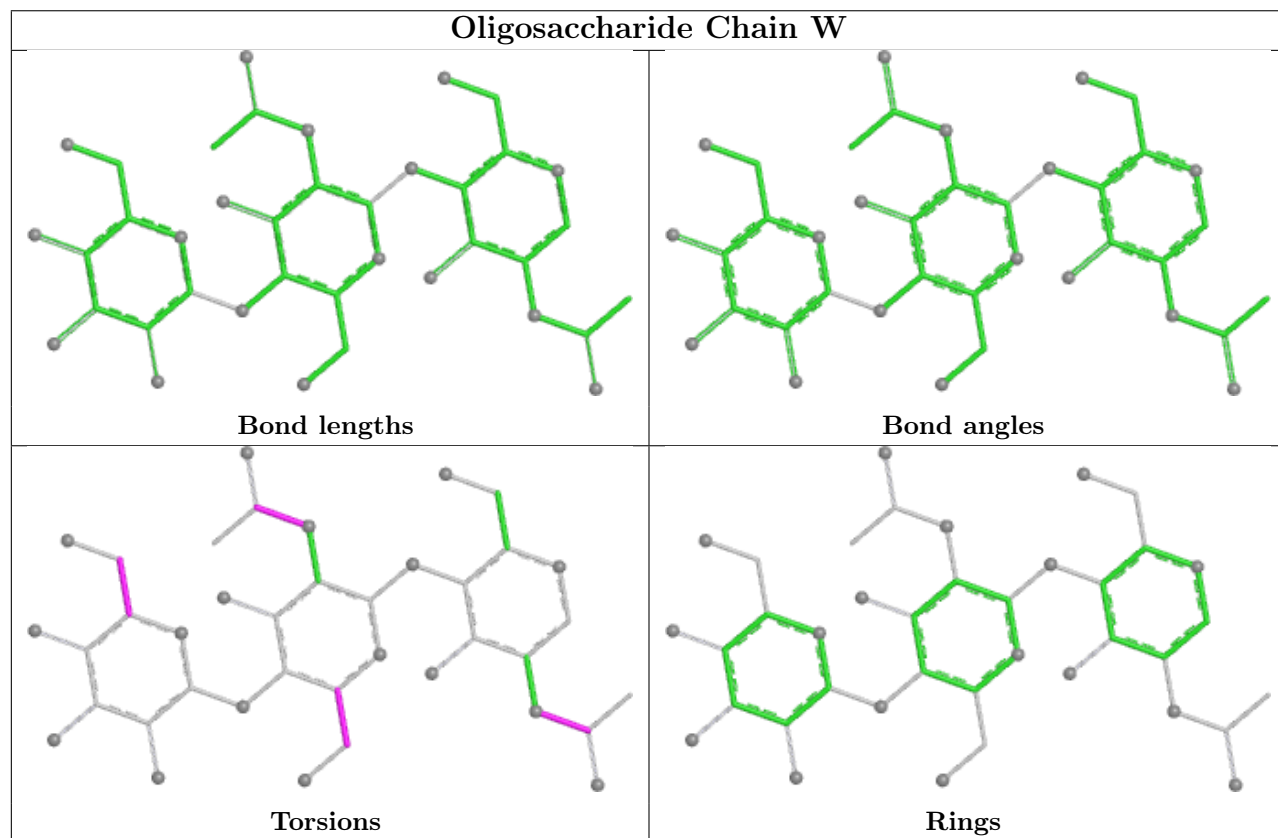
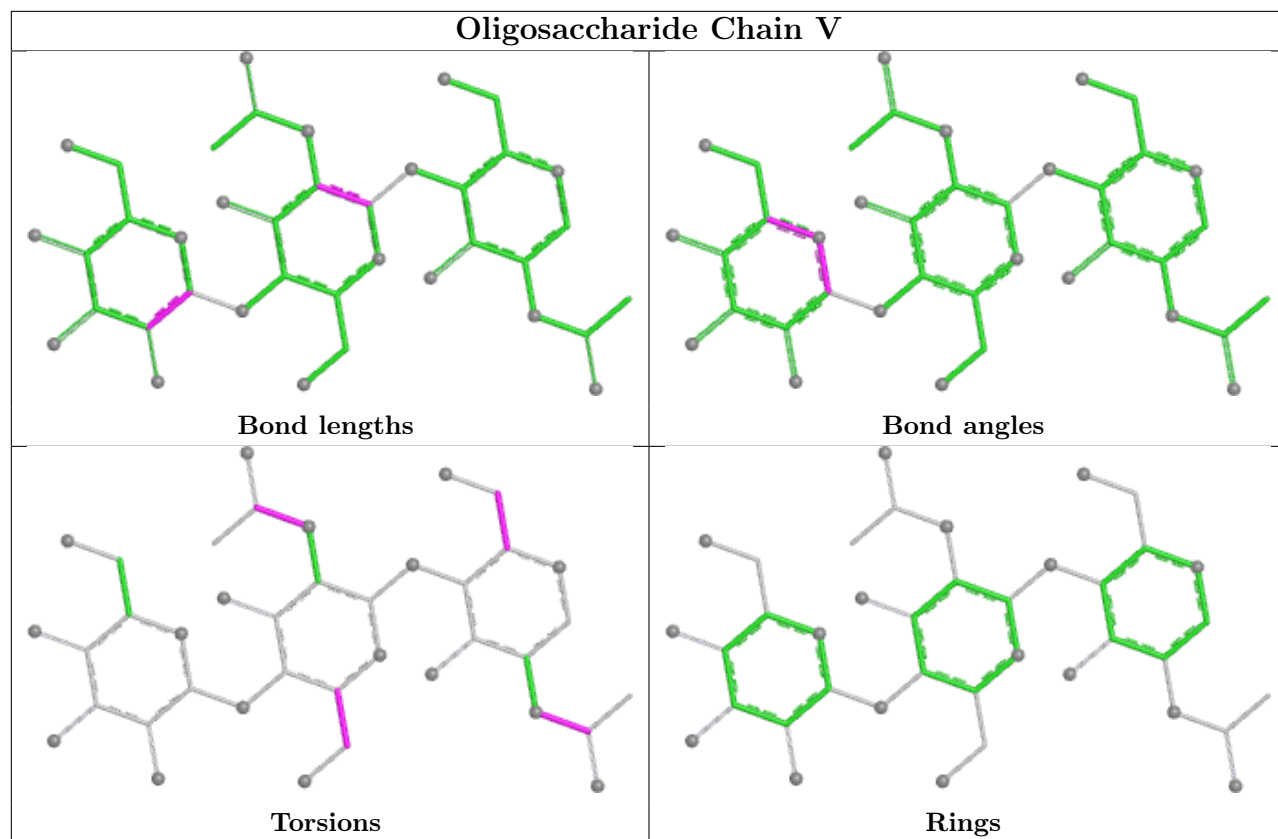
19 monomers are involved in 15 short contacts:

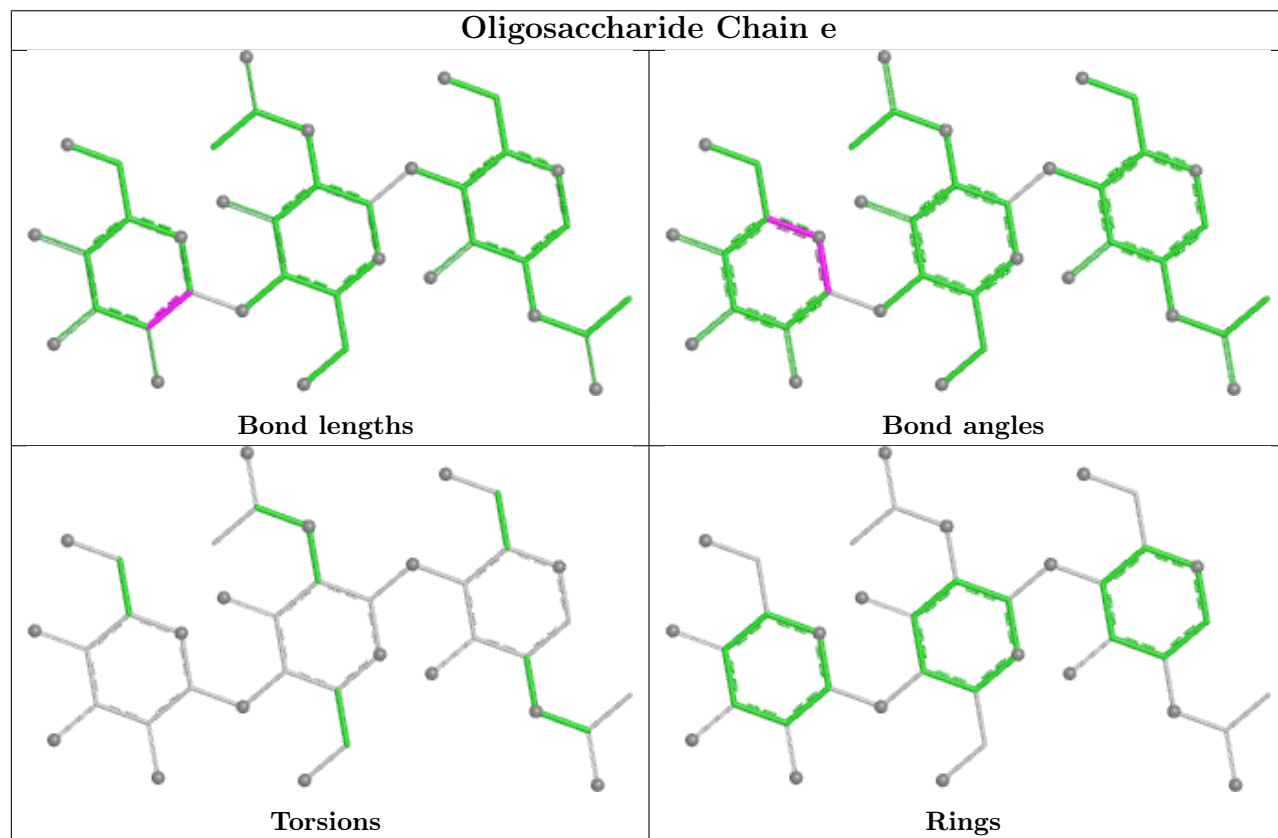
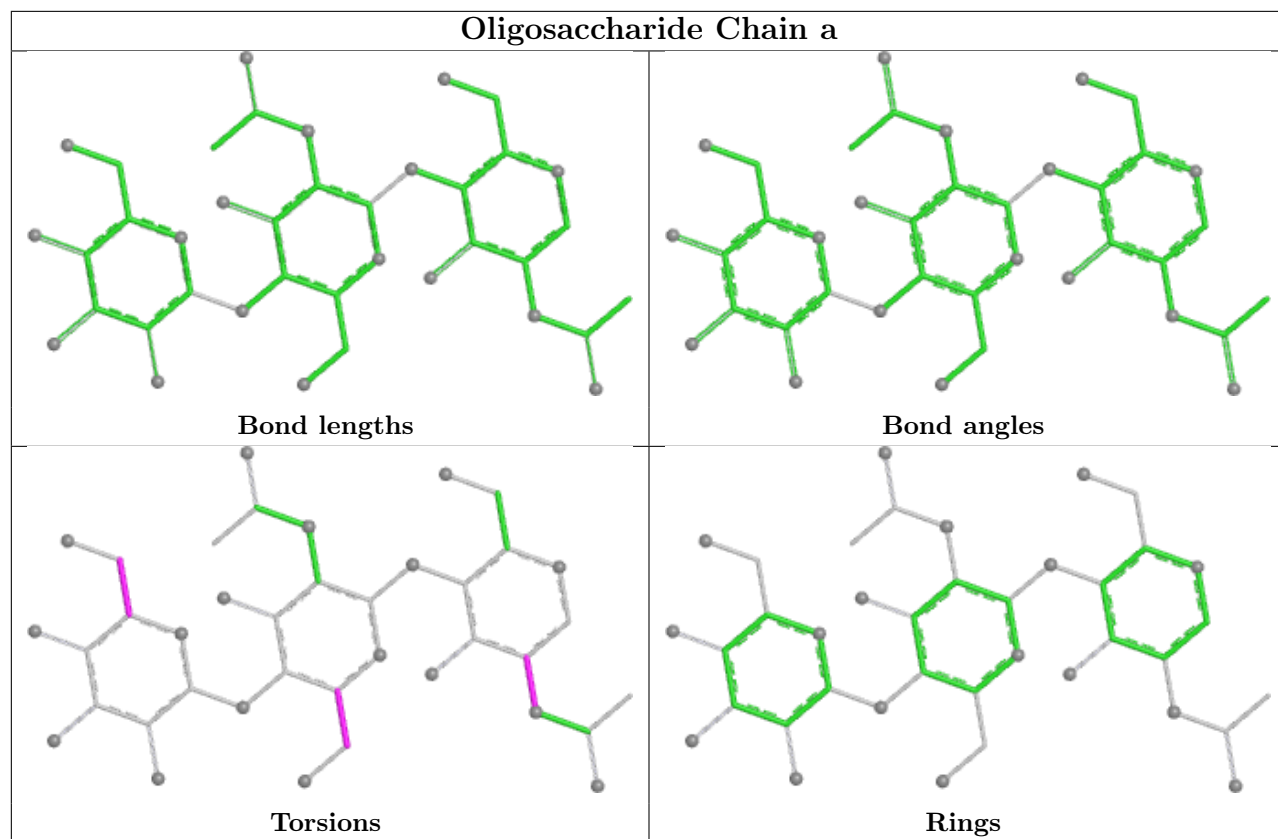
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	a	1	NAG	1	0
4	W	2	NAG	1	0
5	K	2	NAG	1	0
5	K	1	NAG	1	0
4	v	3	BMA	1	0
5	l	2	NAG	2	0
4	e	1	NAG	1	0
4	v	2	NAG	2	0
4	W	3	BMA	1	0
5	Z	2	NAG	1	0
5	k	2	NAG	1	0
5	O	1	NAG	1	0
5	k	1	NAG	1	0
5	Y	2	NAG	1	0
5	p	1	NAG	2	0
5	p	2	NAG	2	0
5	Y	1	NAG	1	0
5	l	1	NAG	1	0
5	Z	1	NAG	2	0

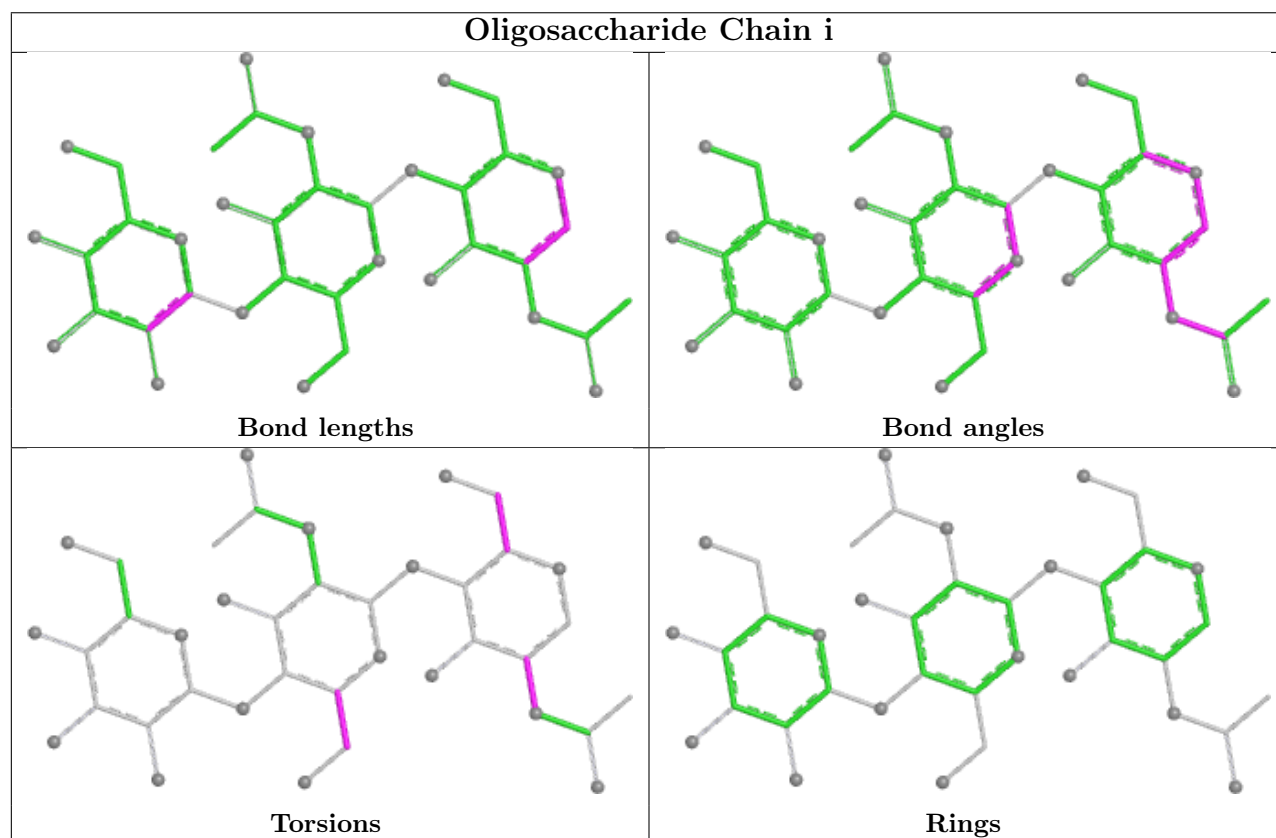
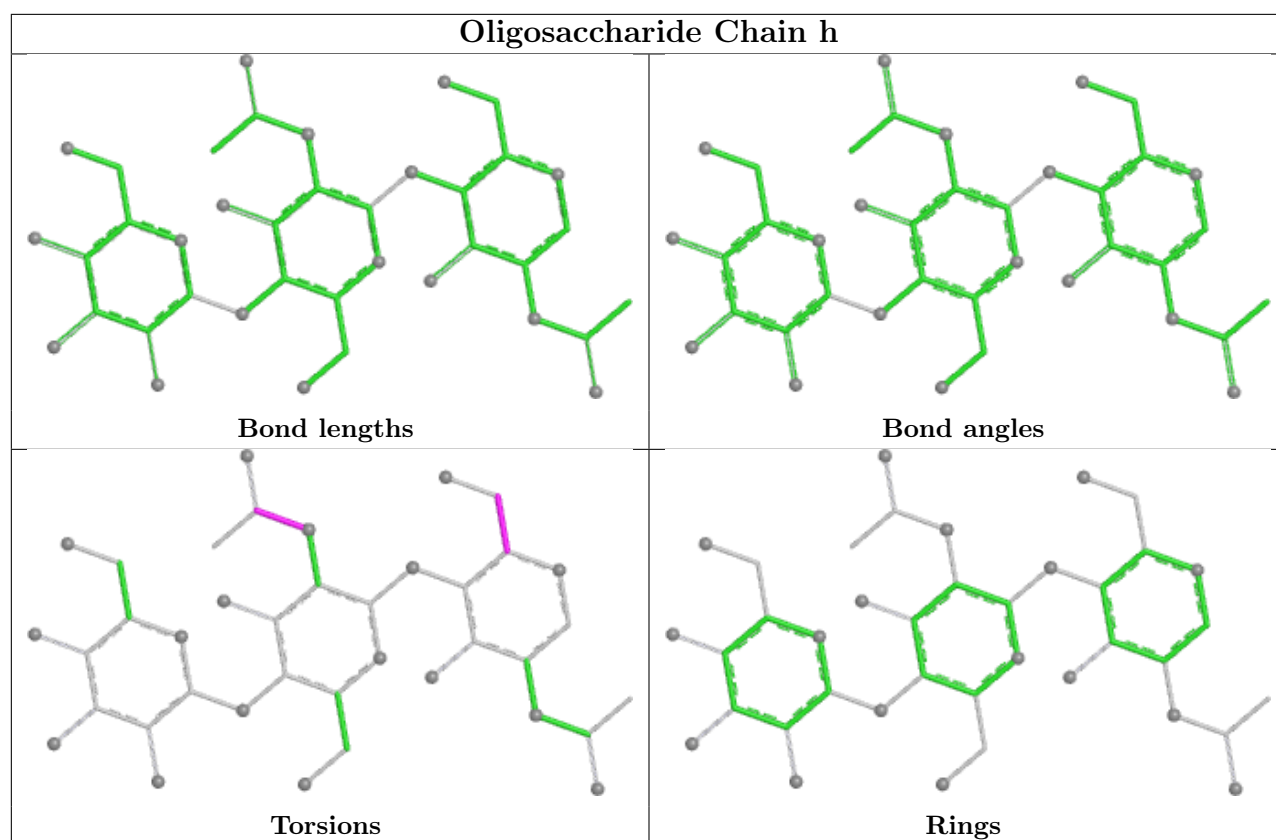
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

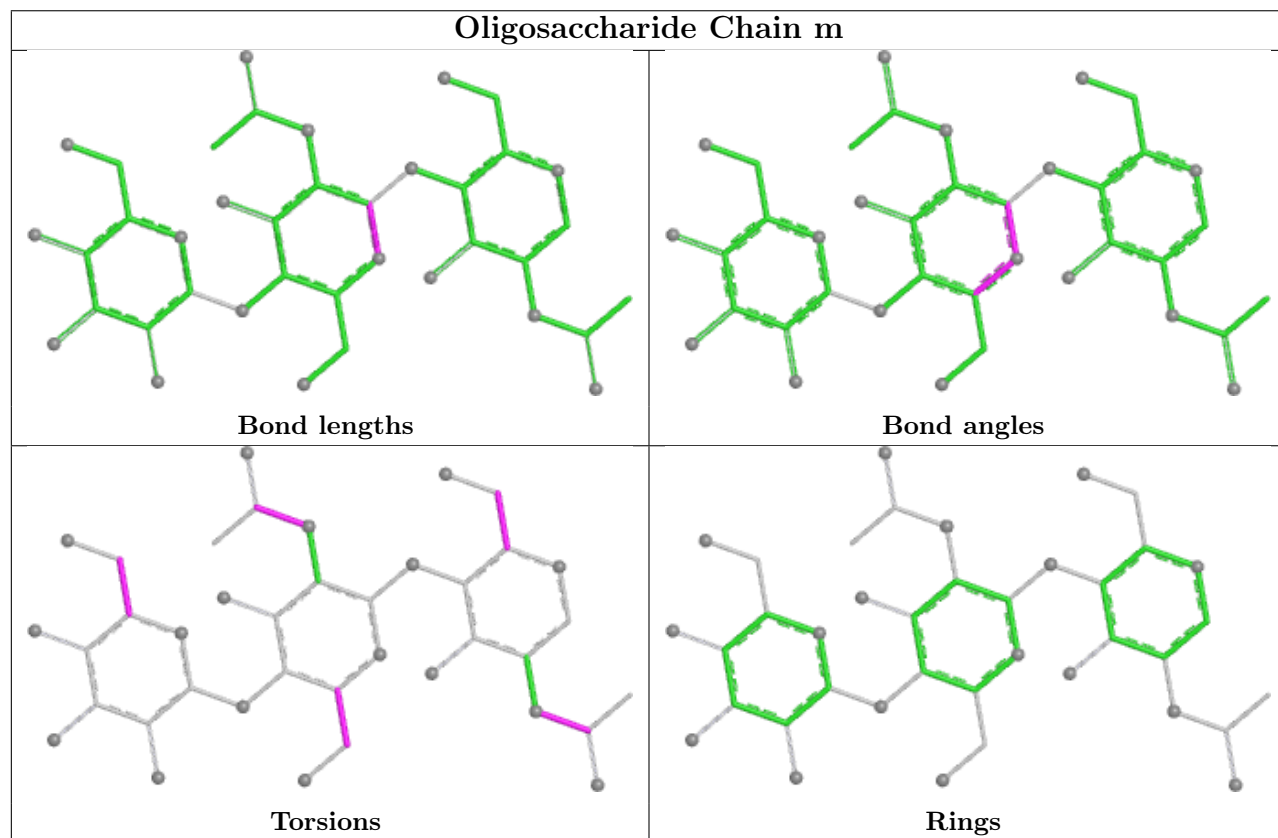
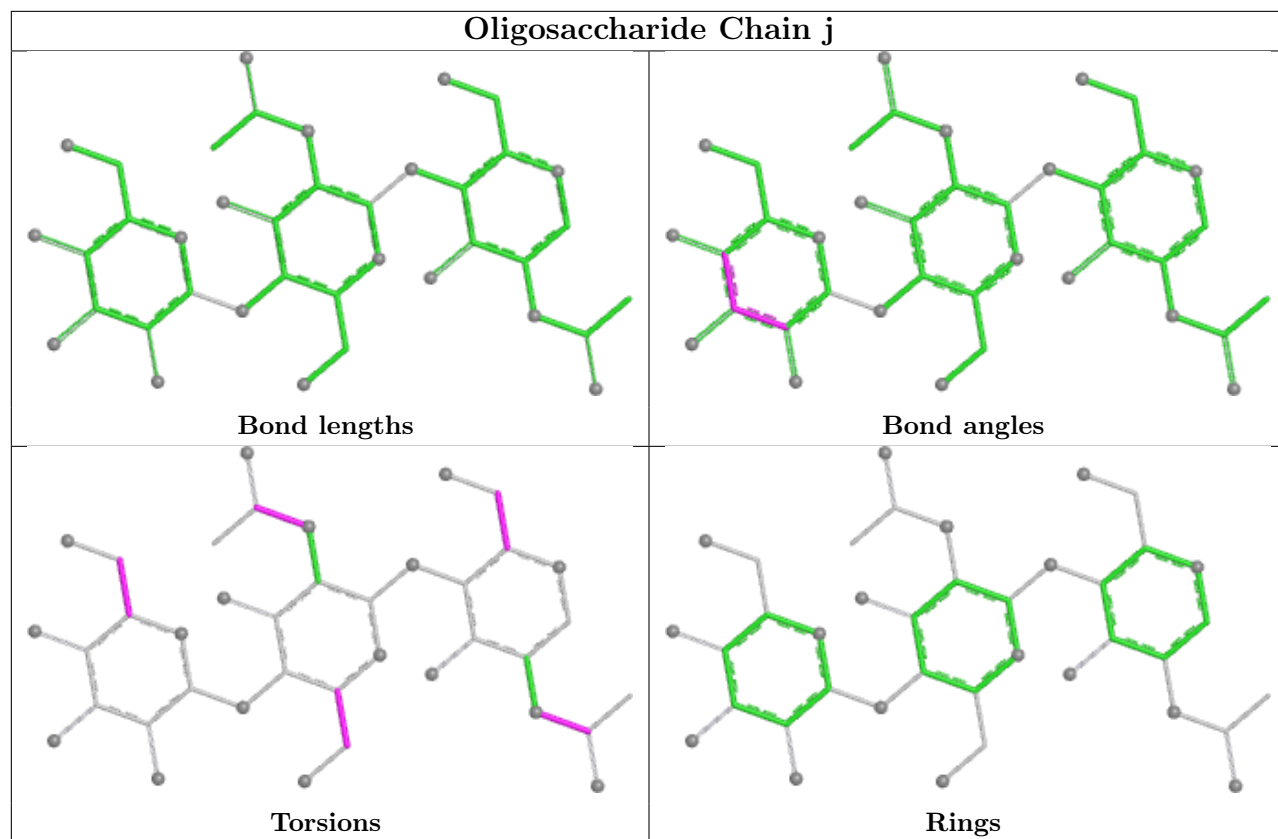


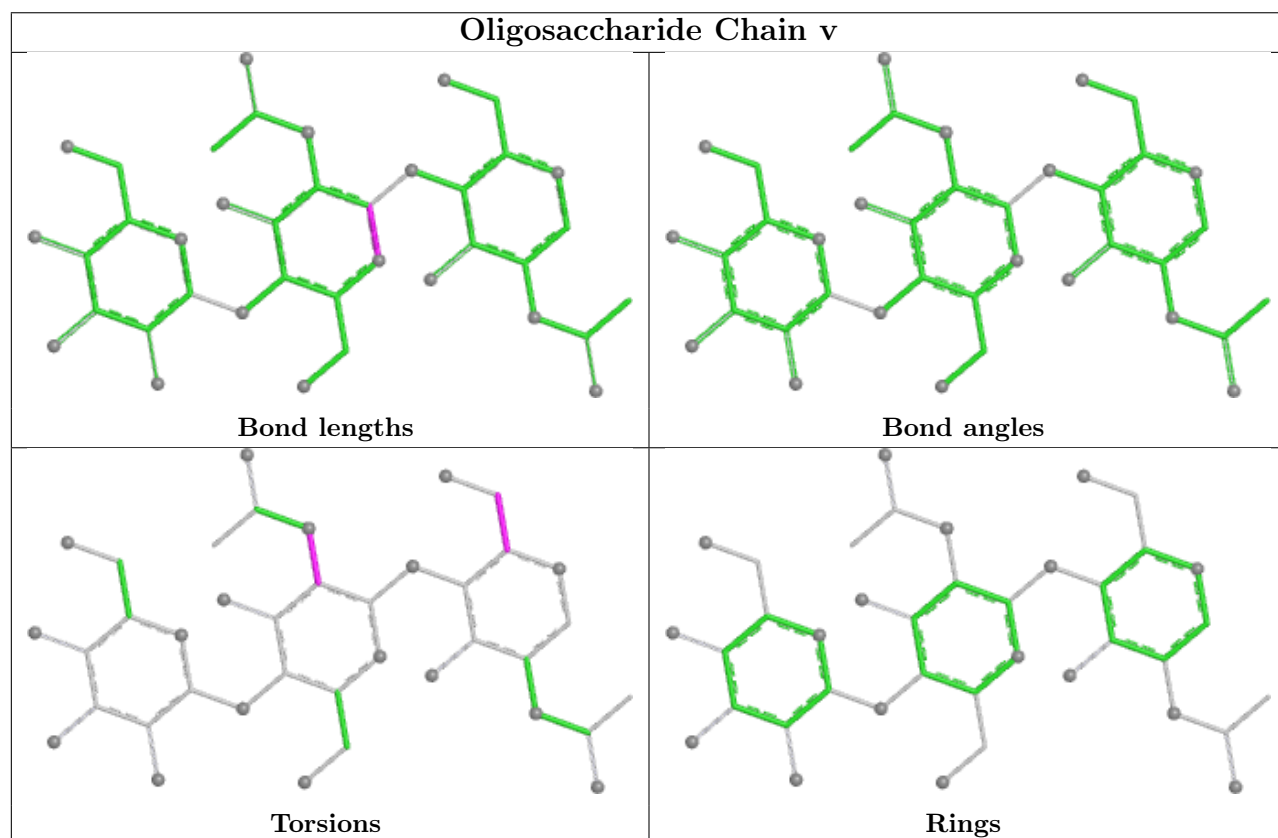
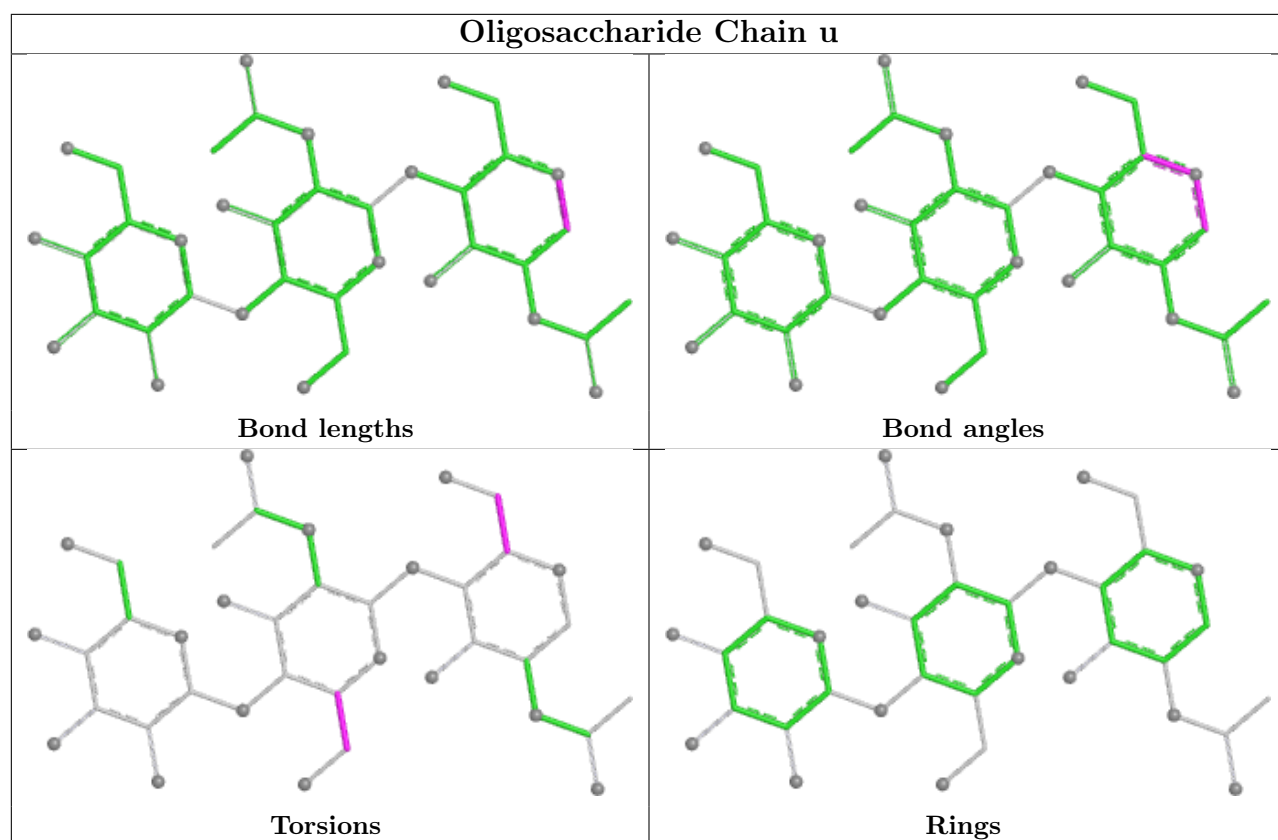


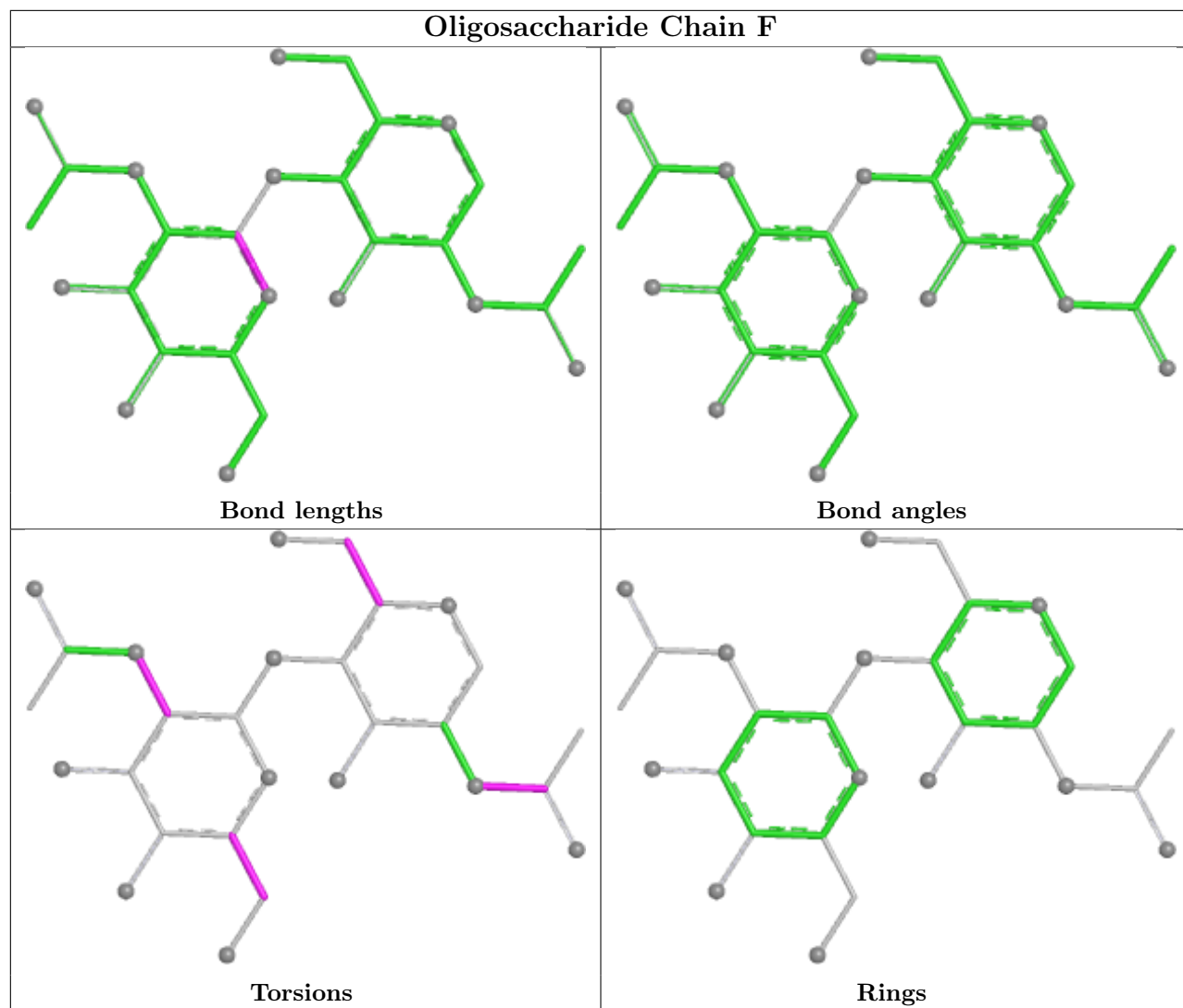


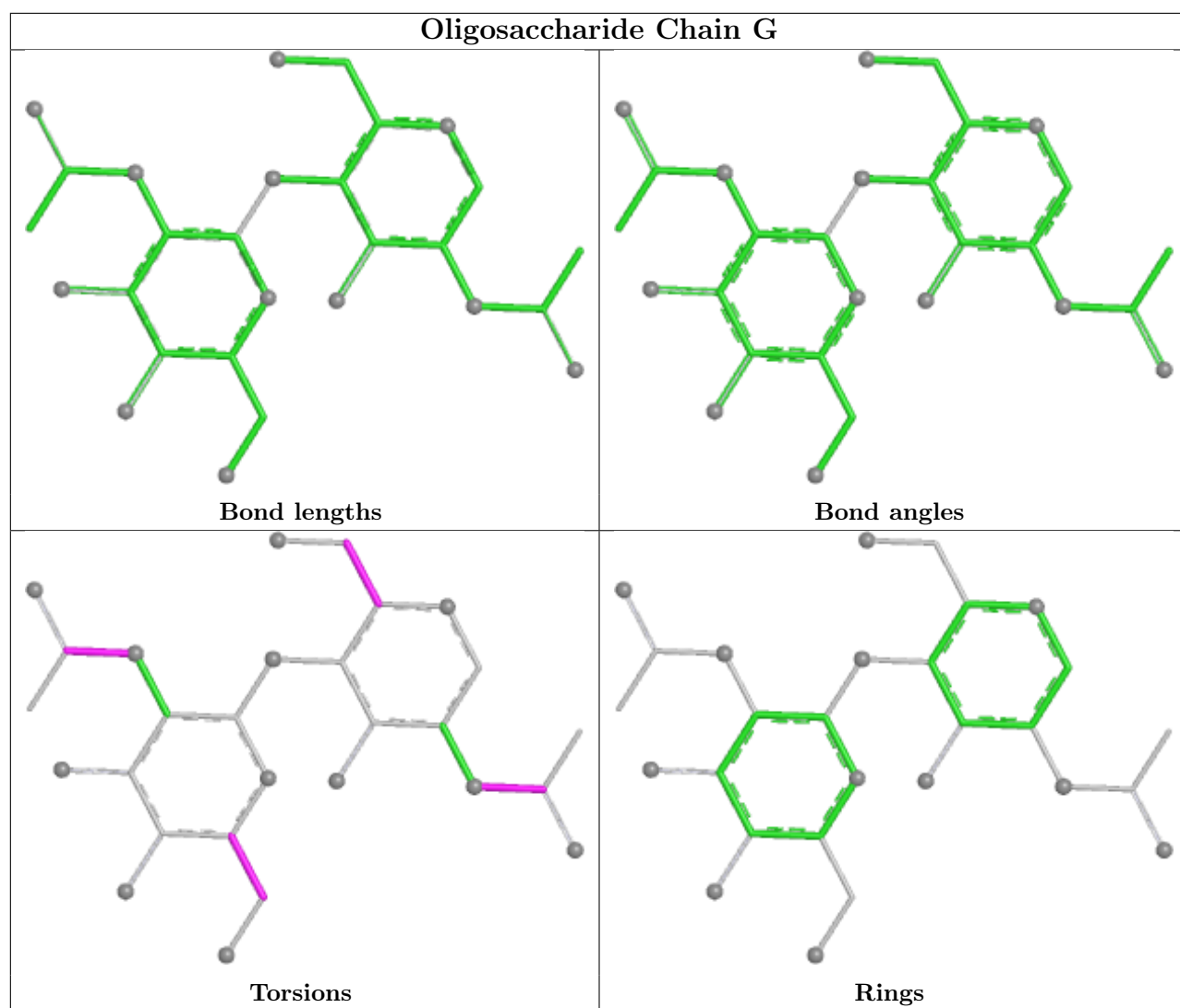


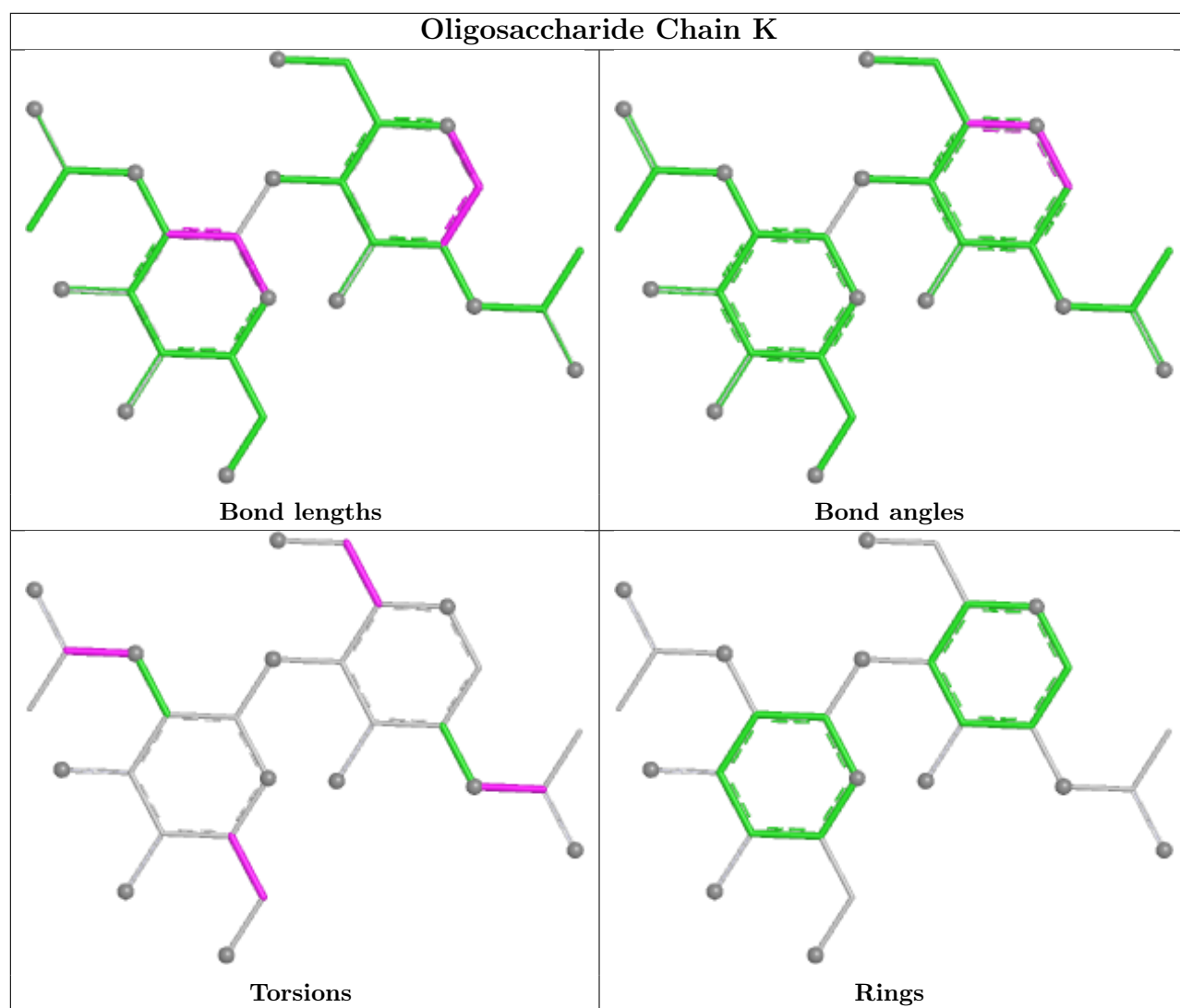


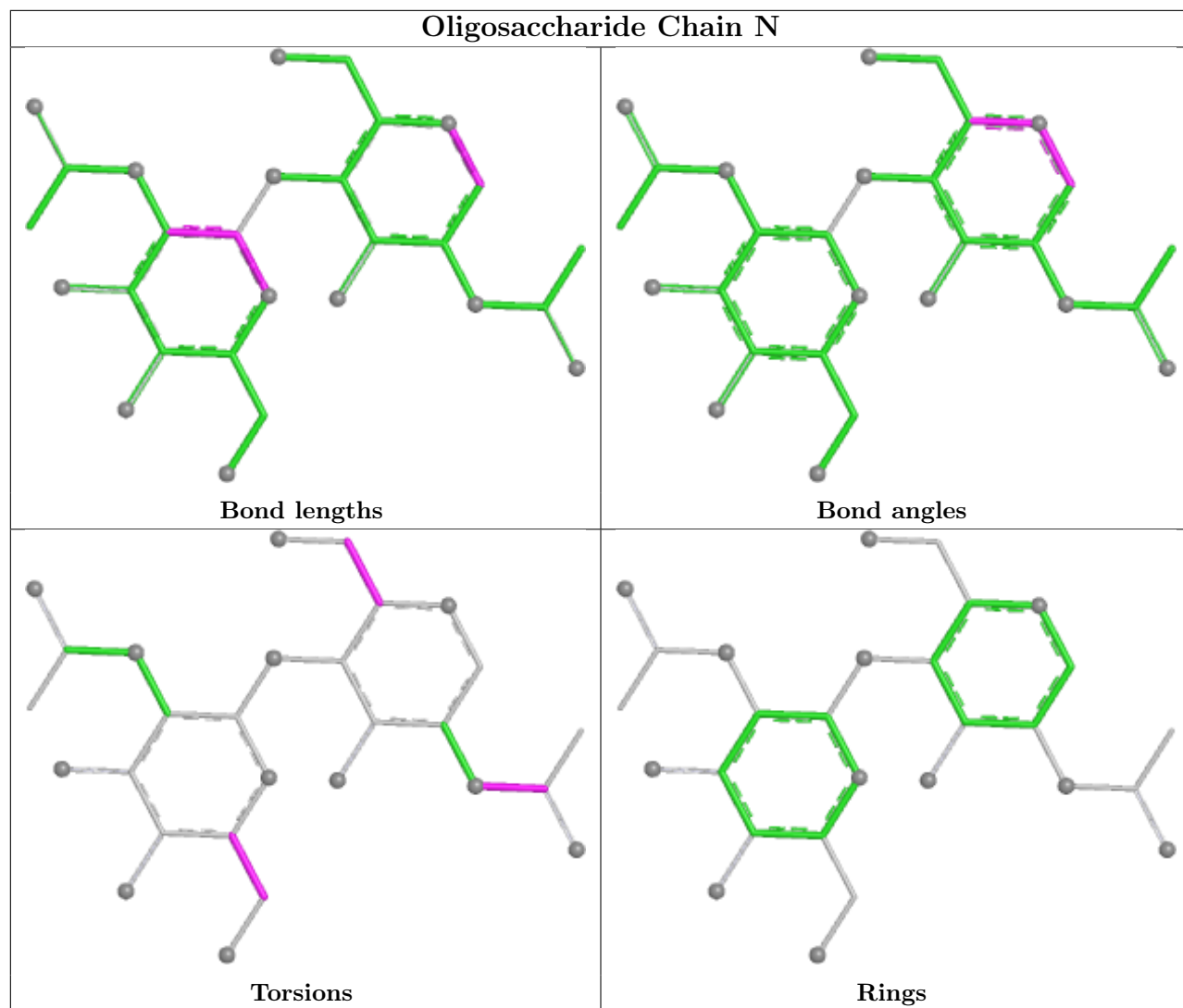


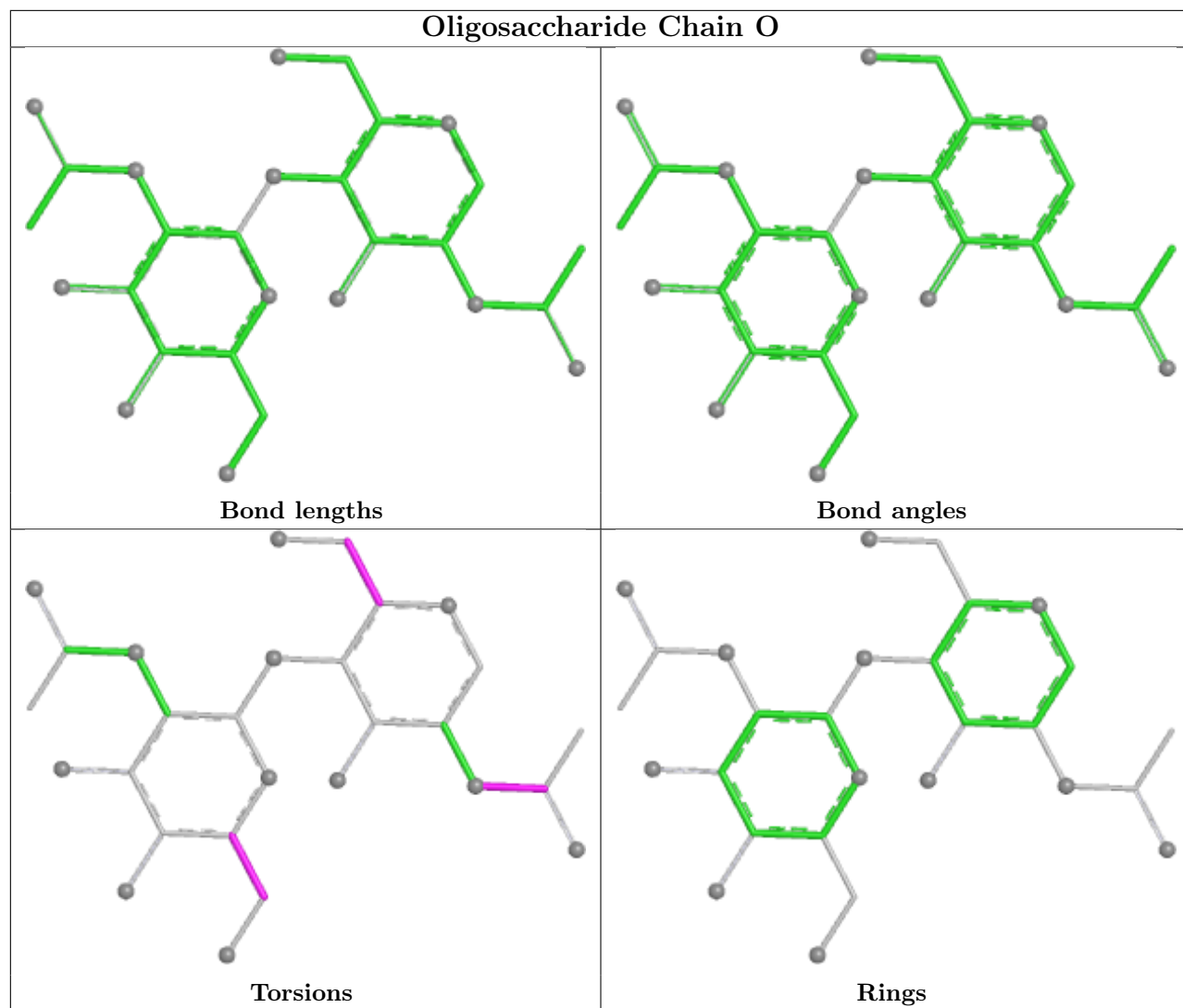


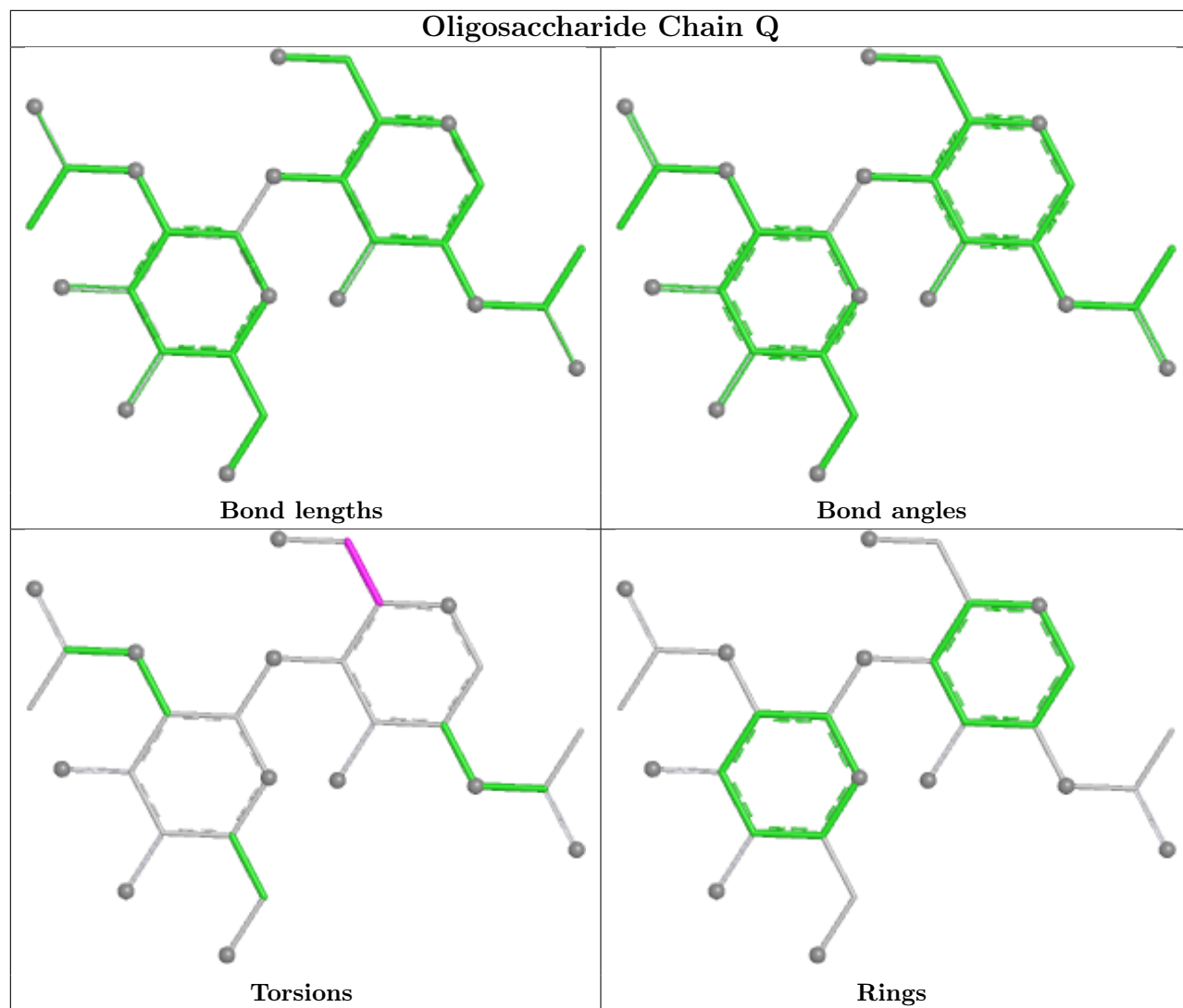


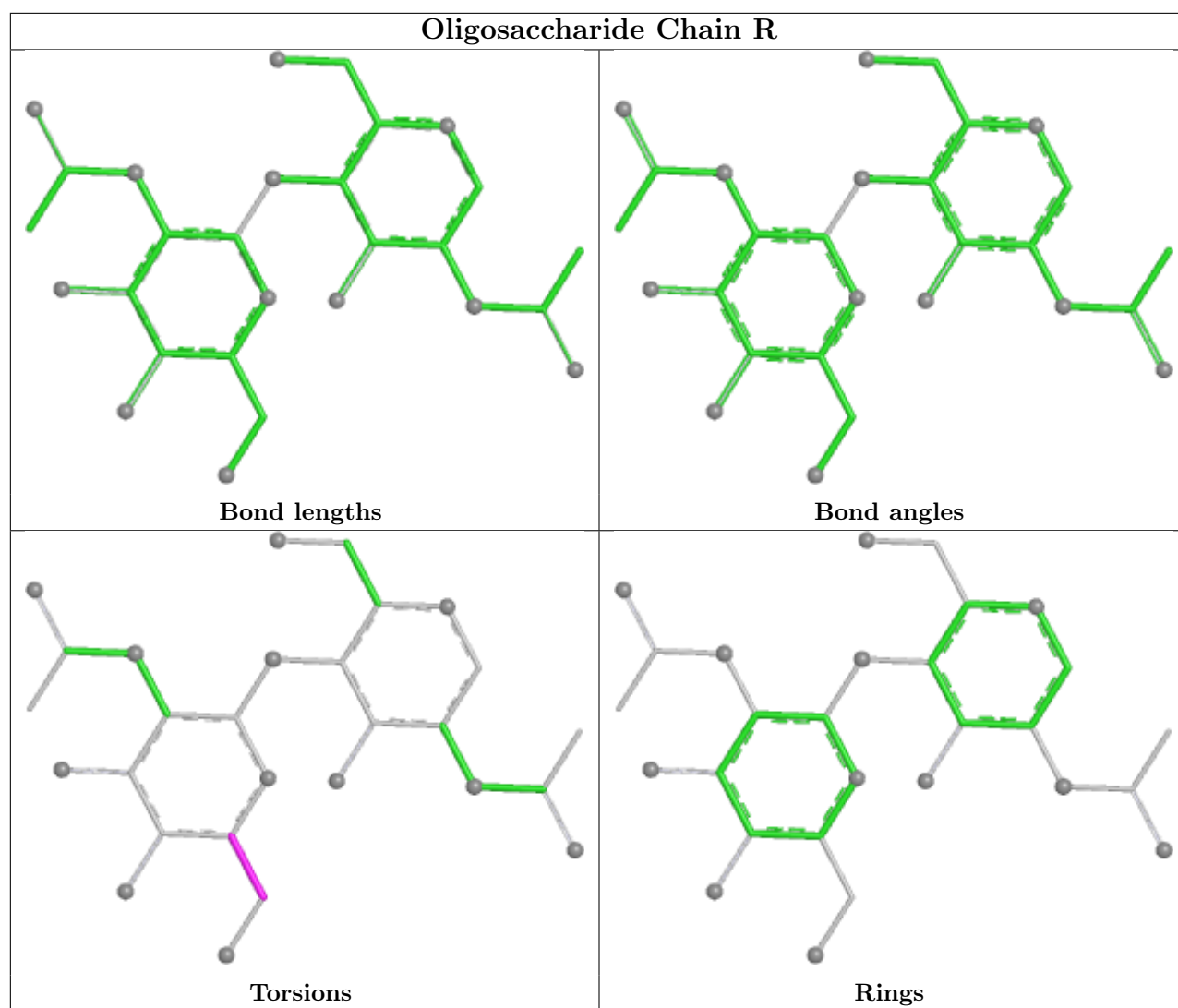


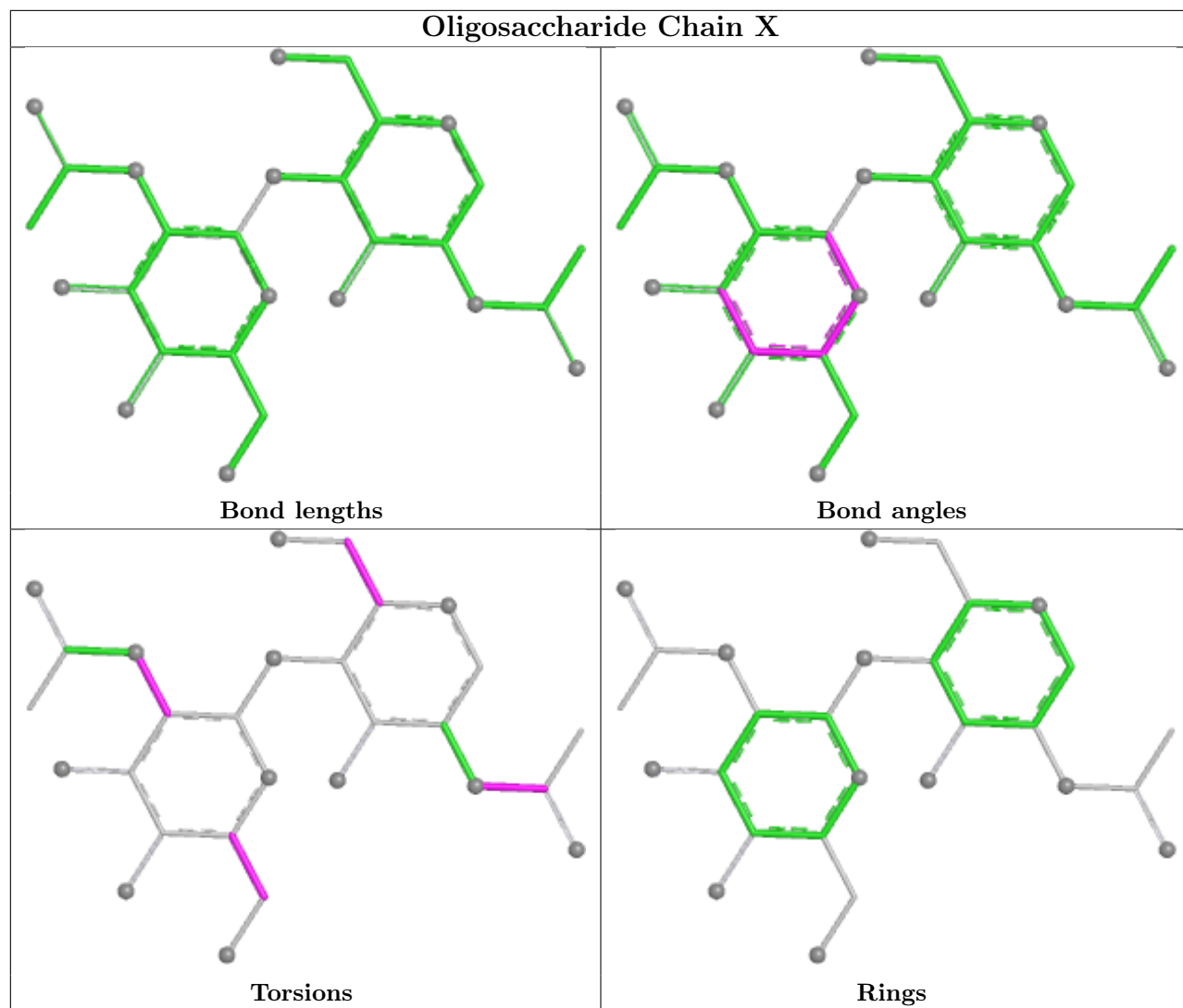


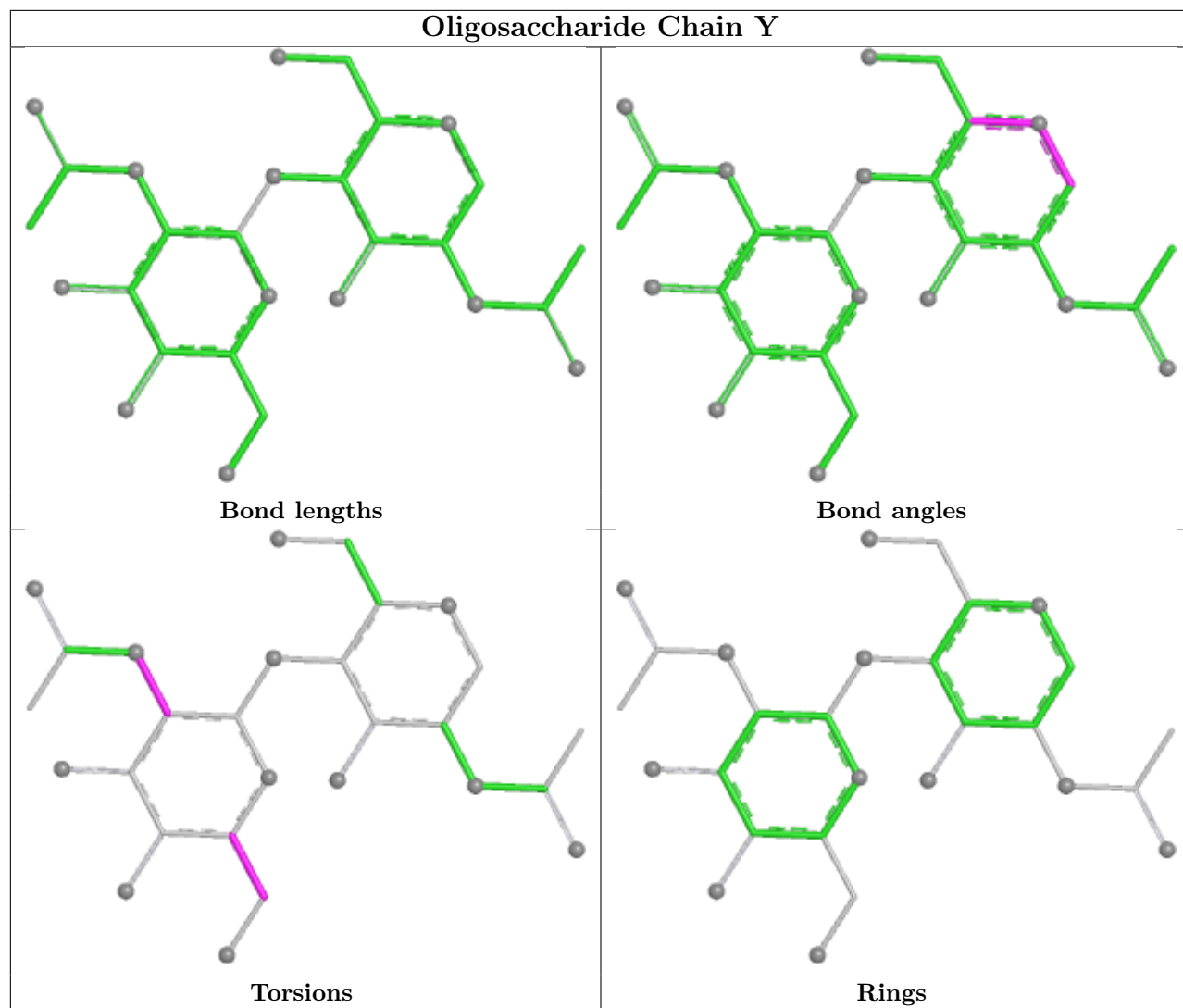


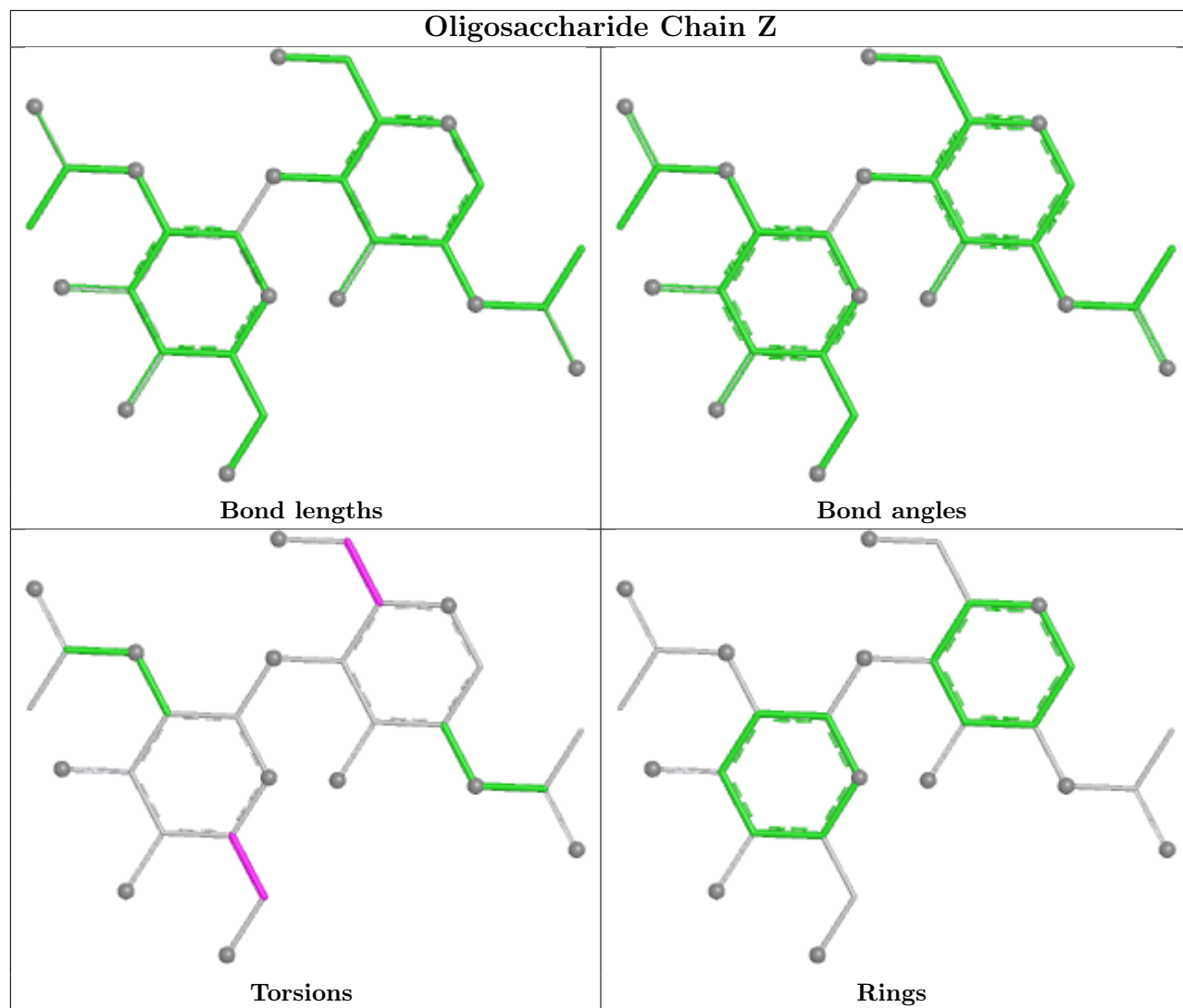


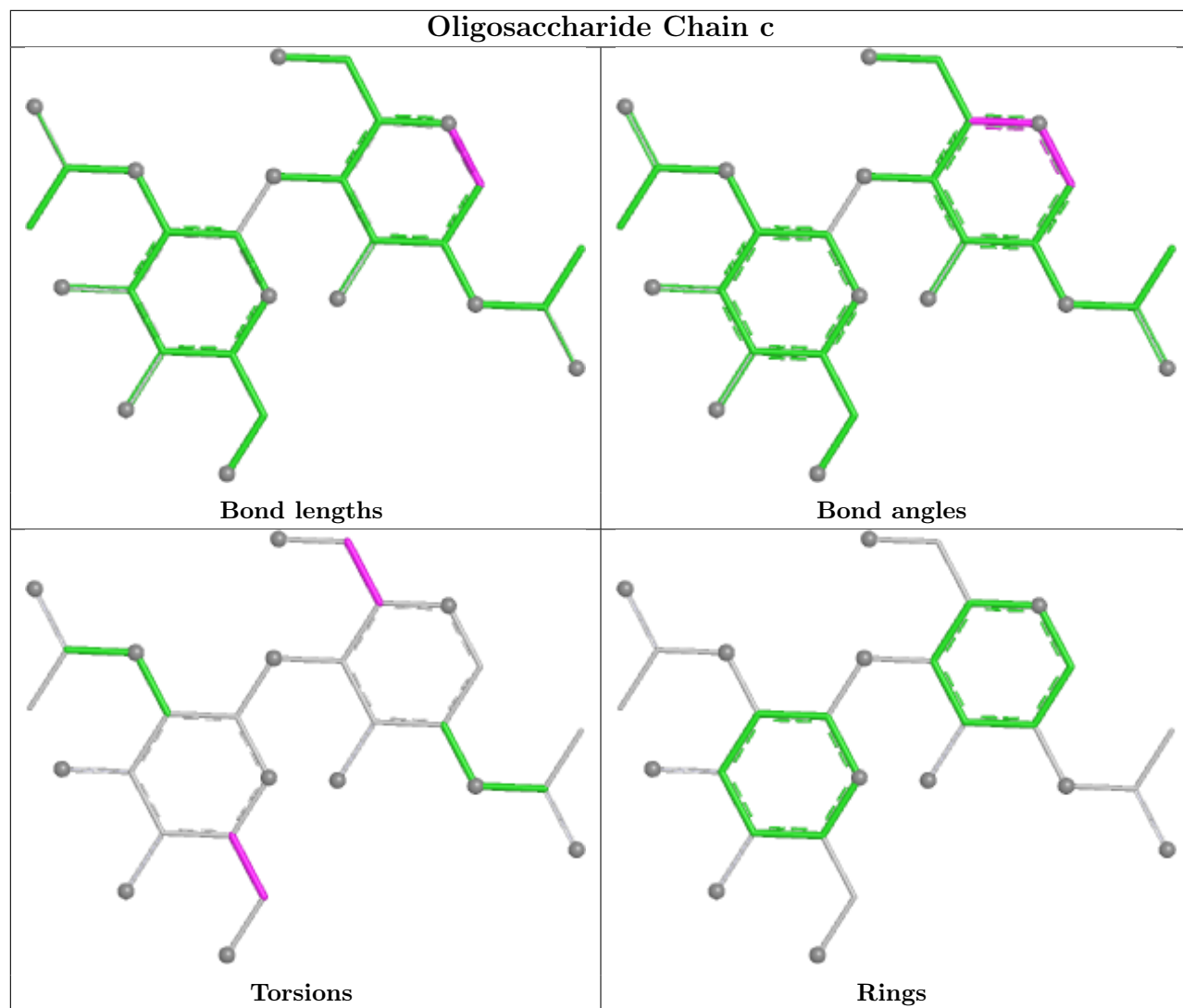


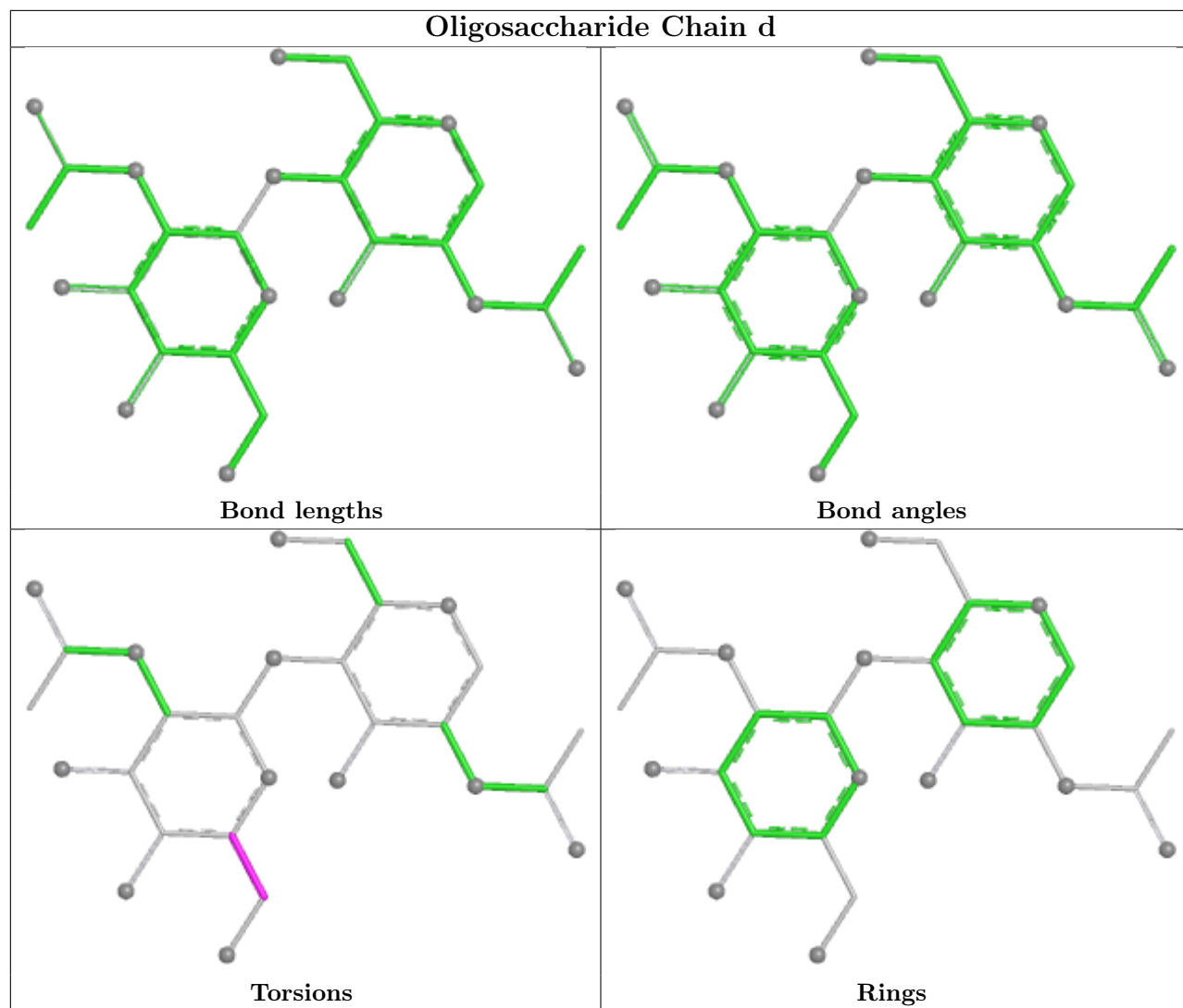


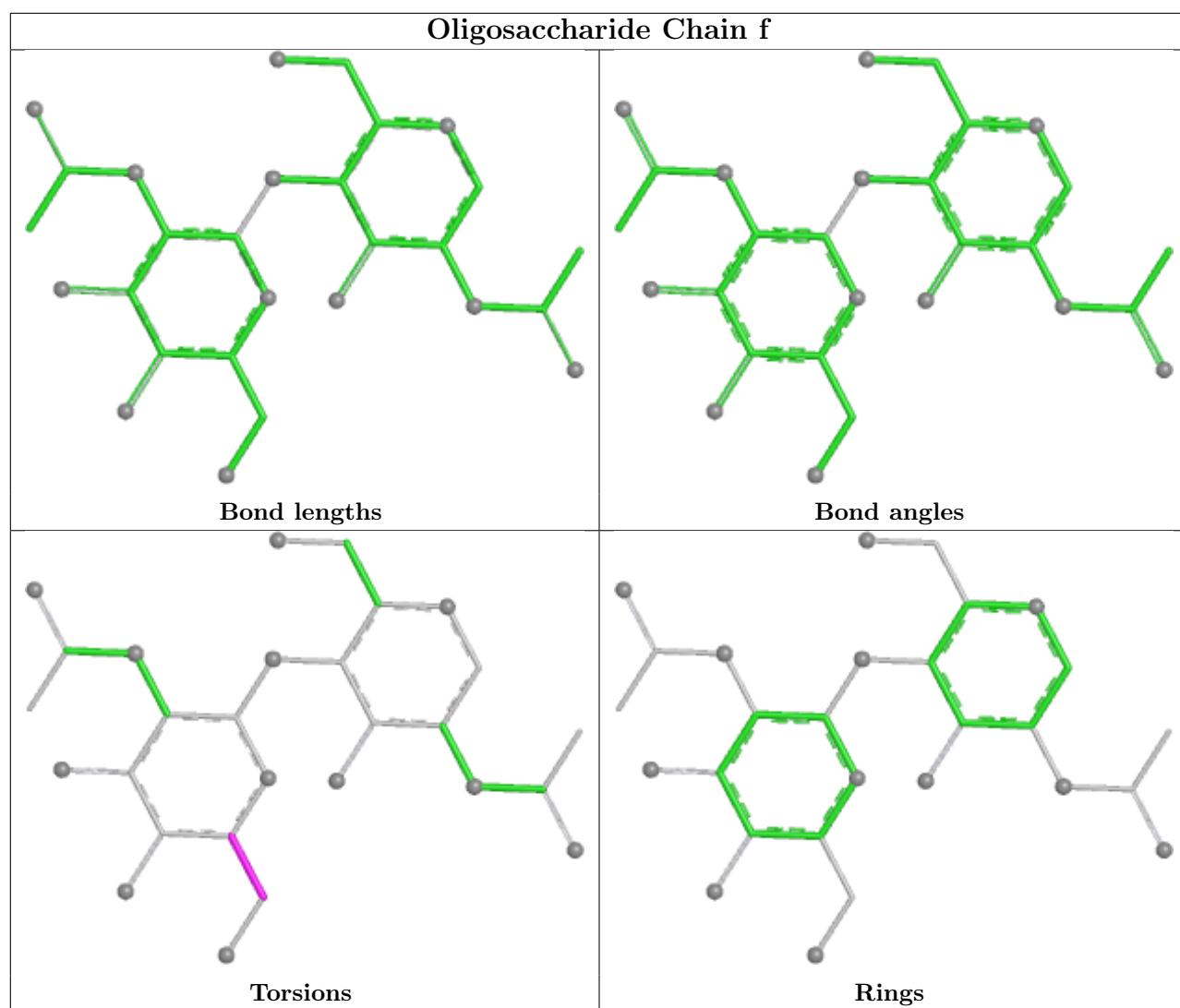


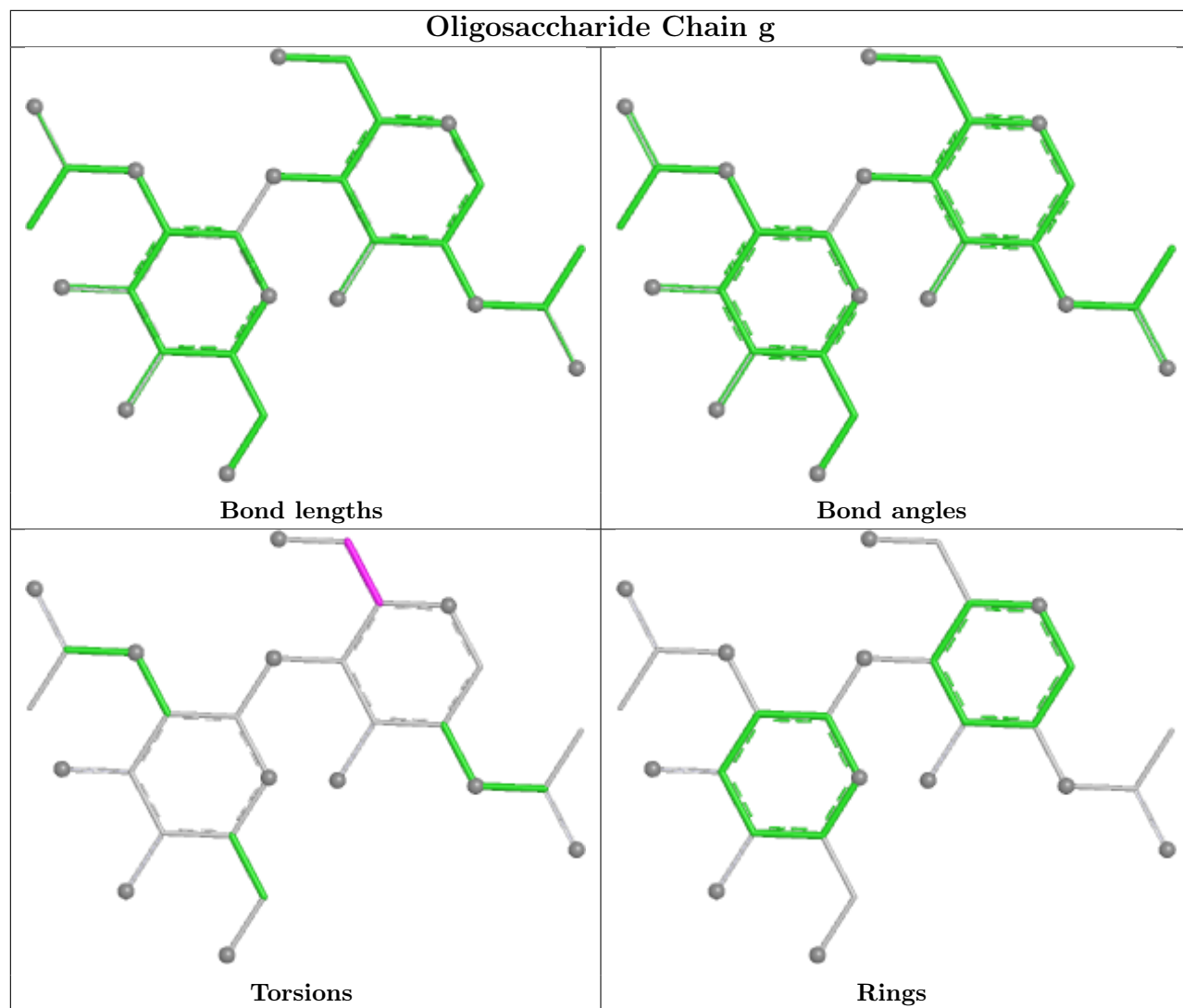


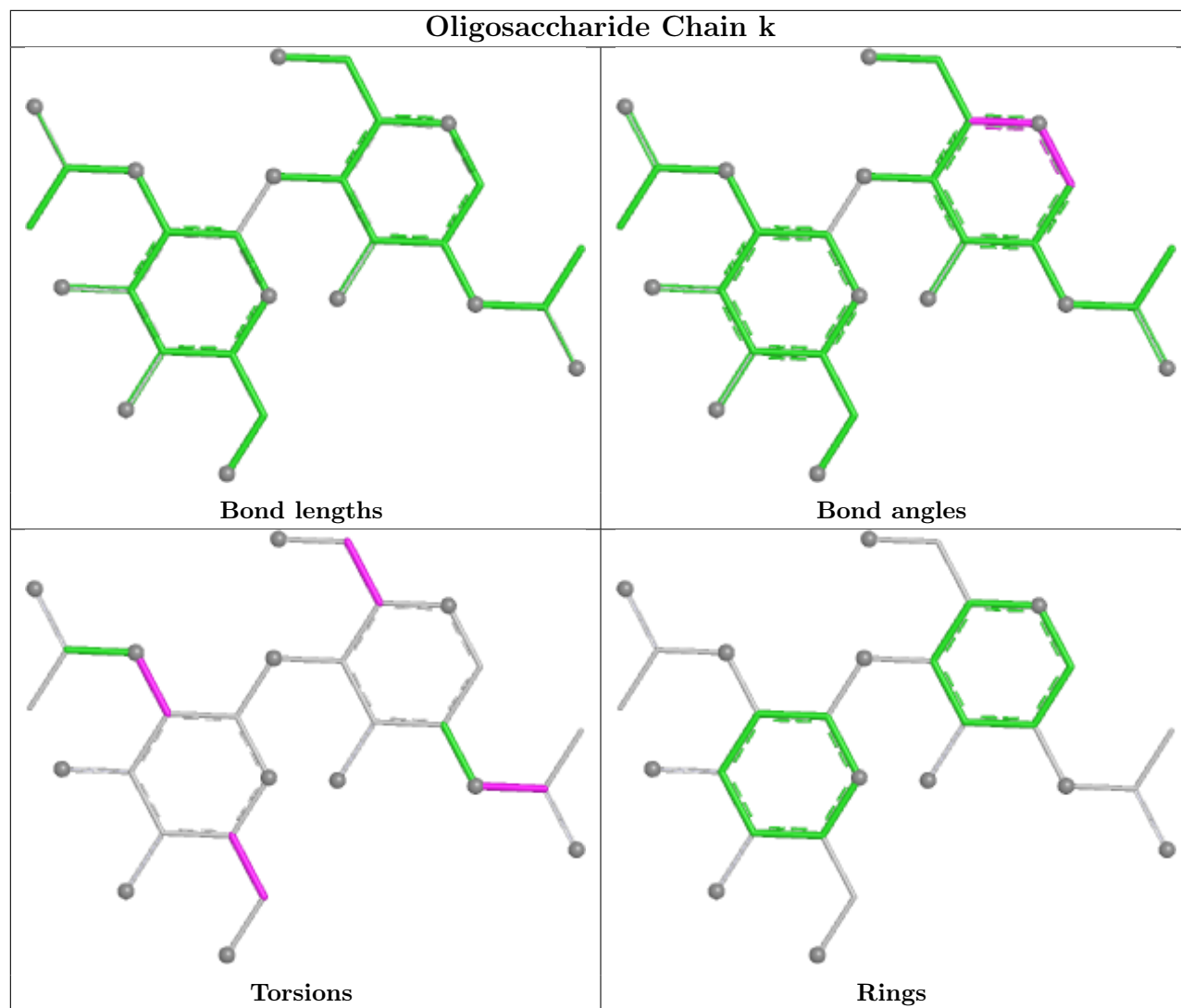


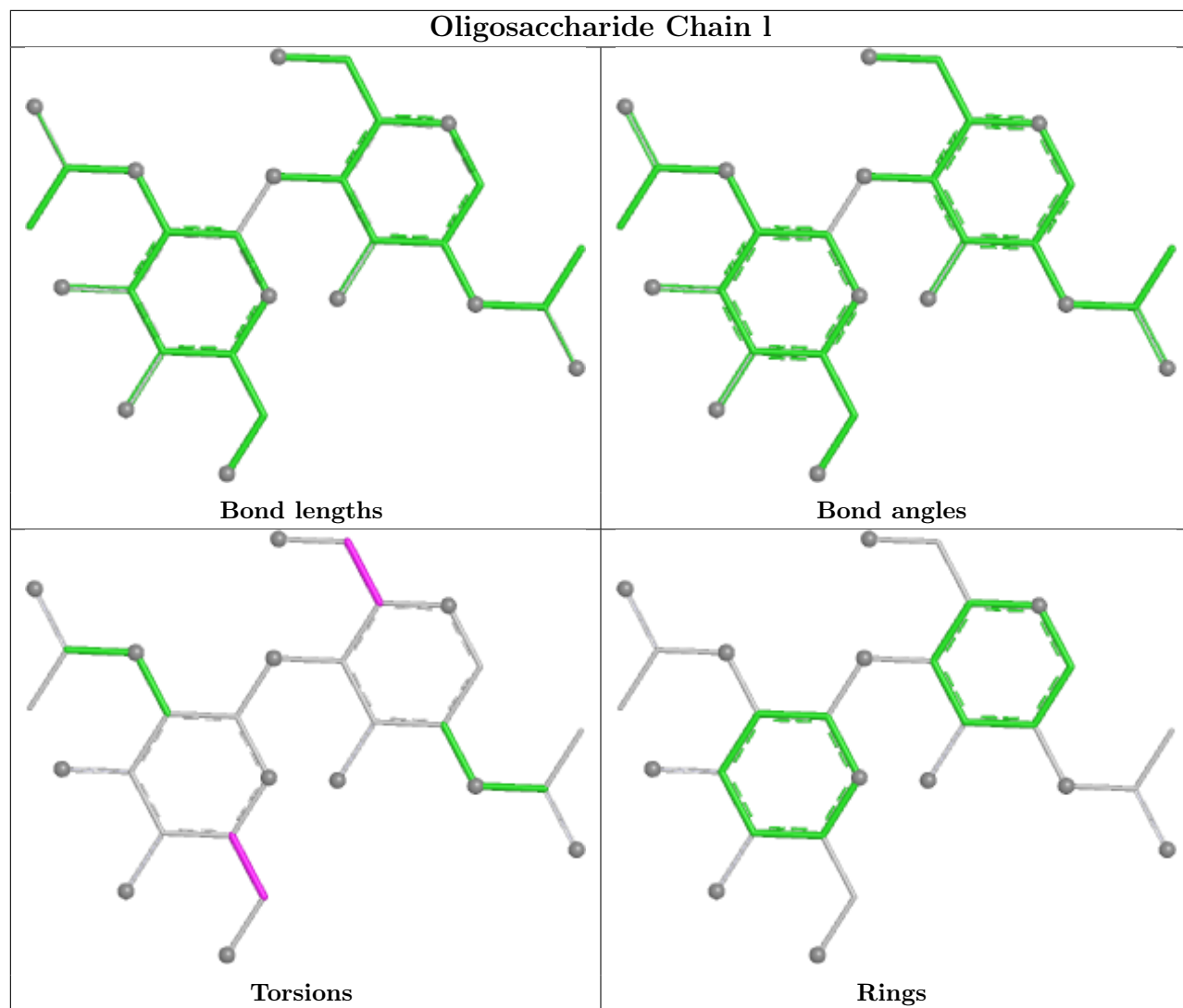


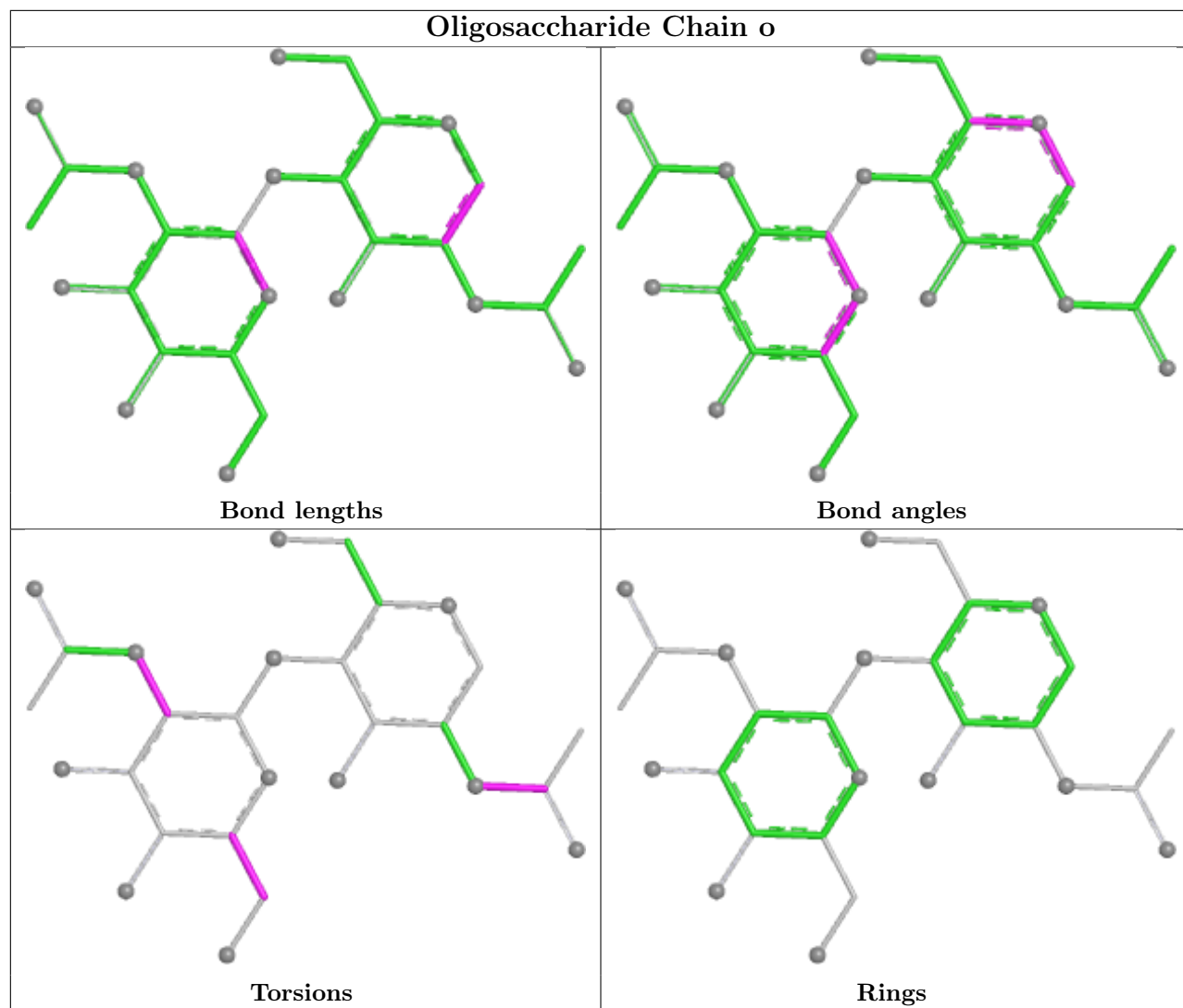


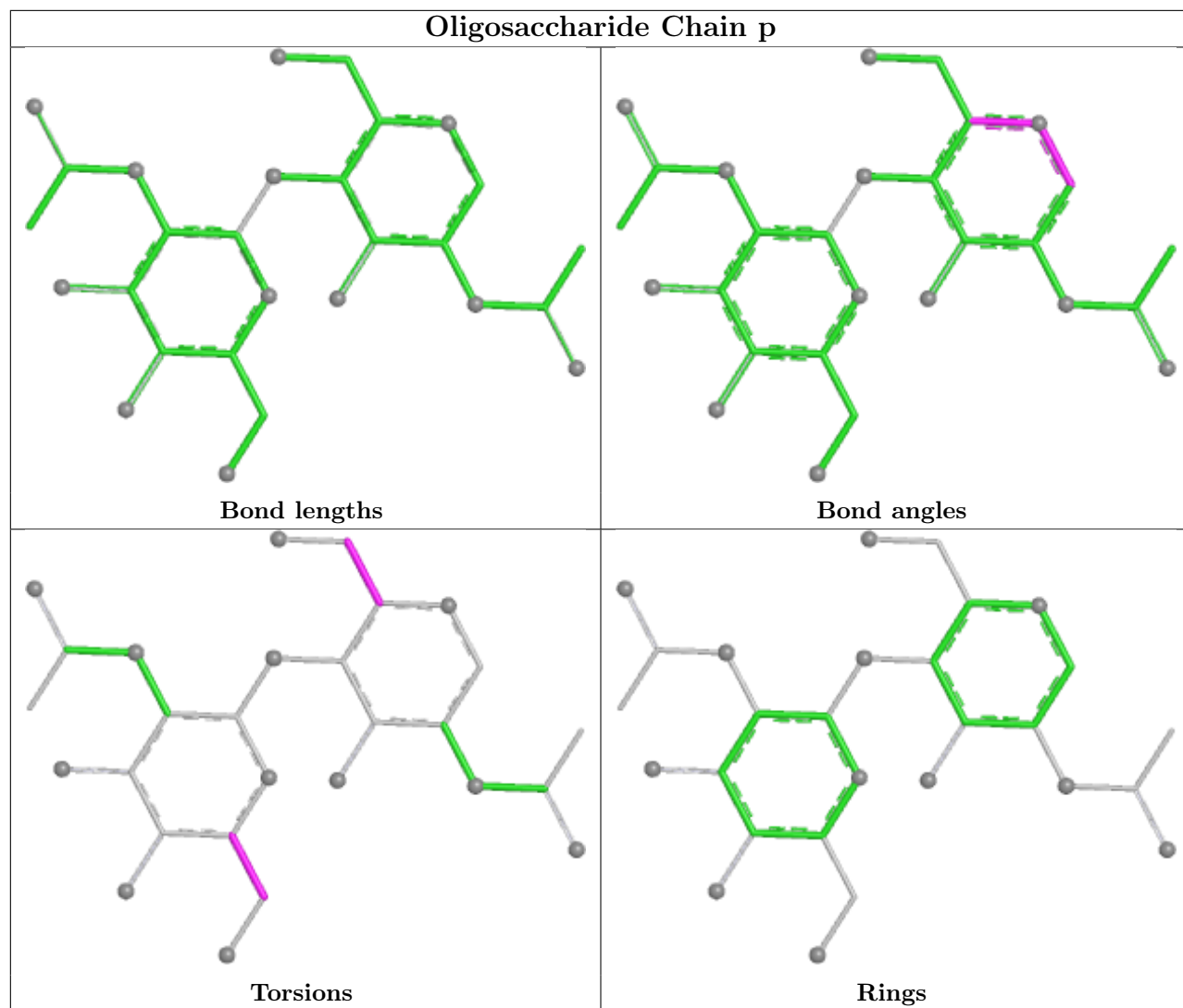


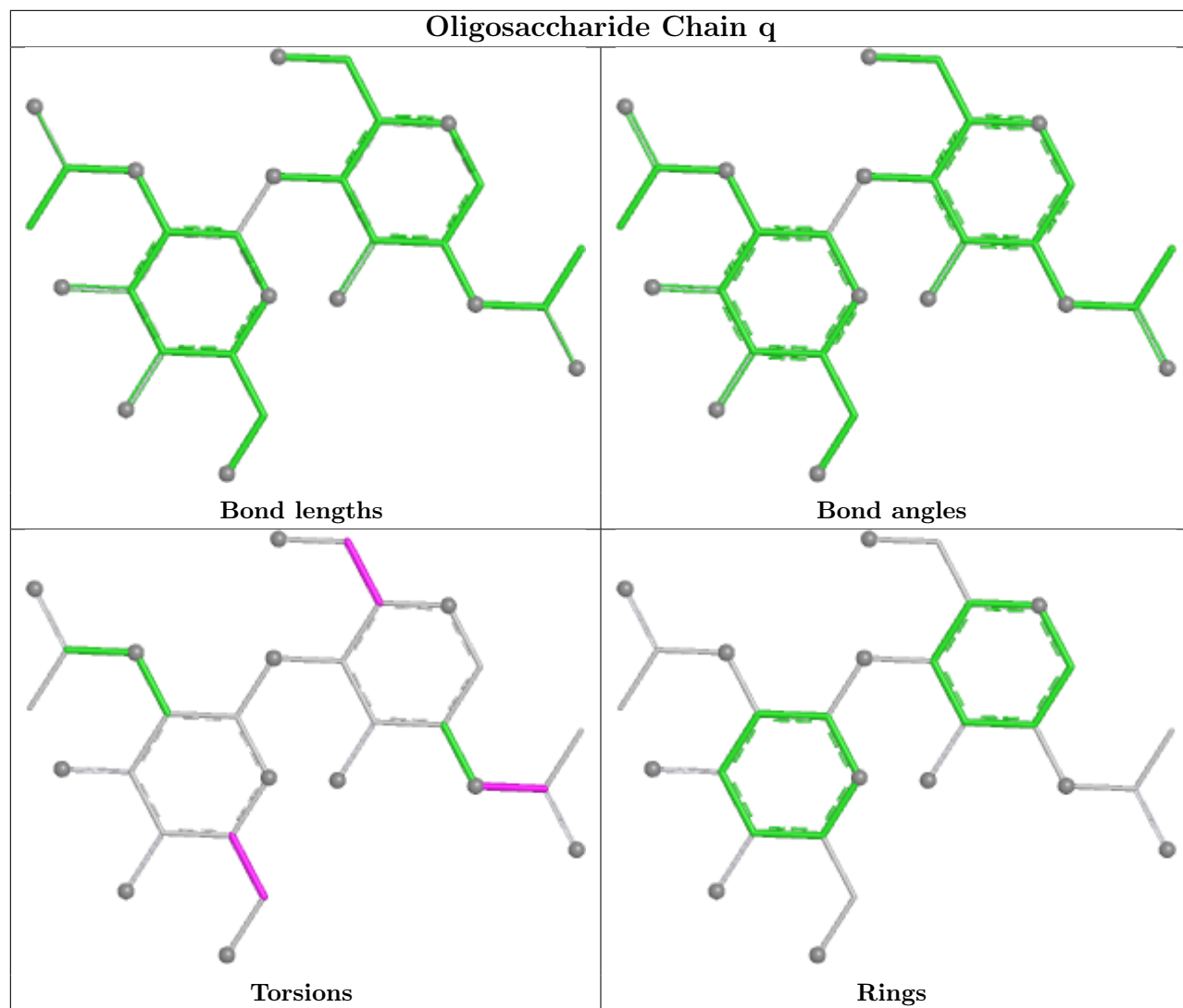


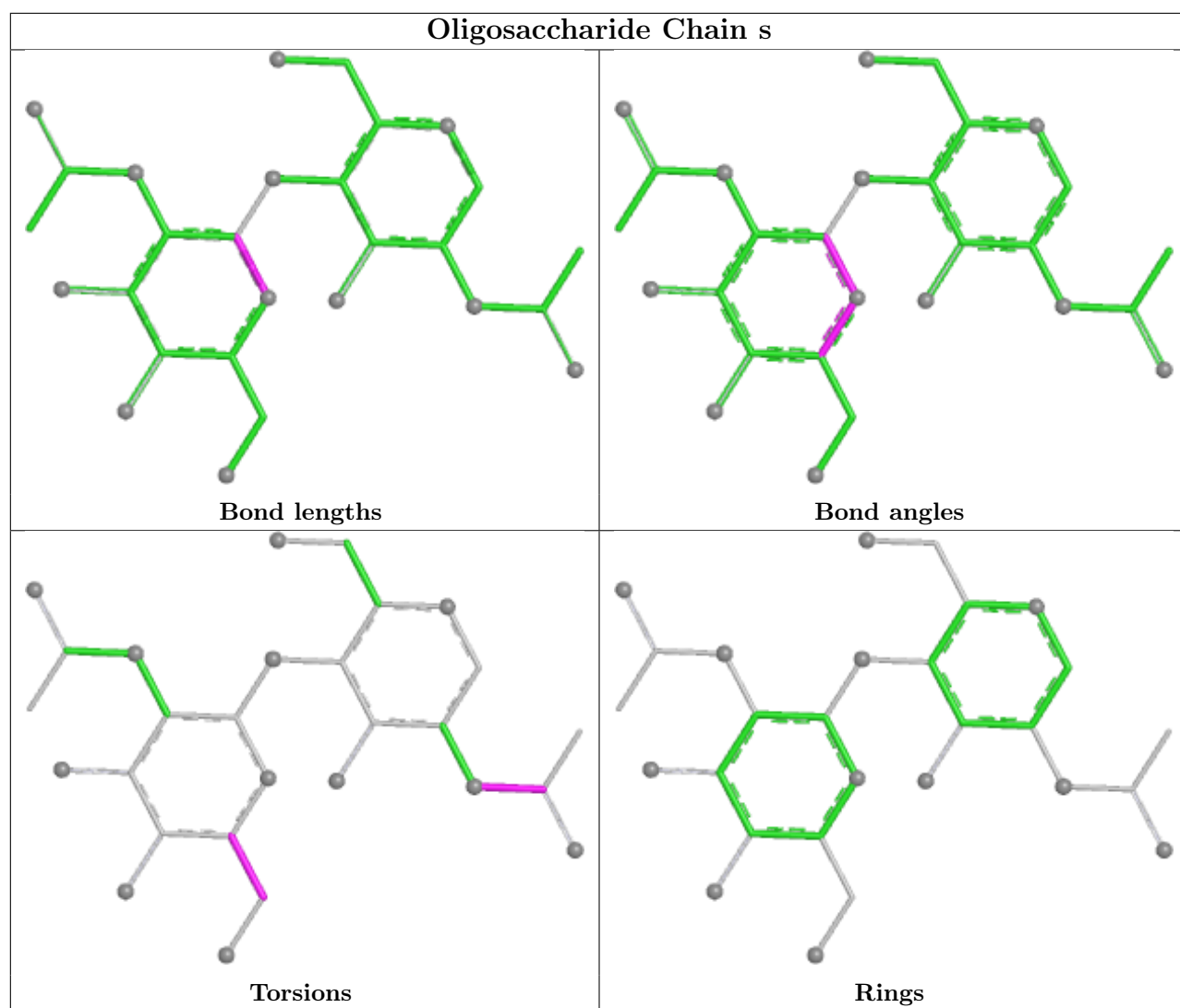


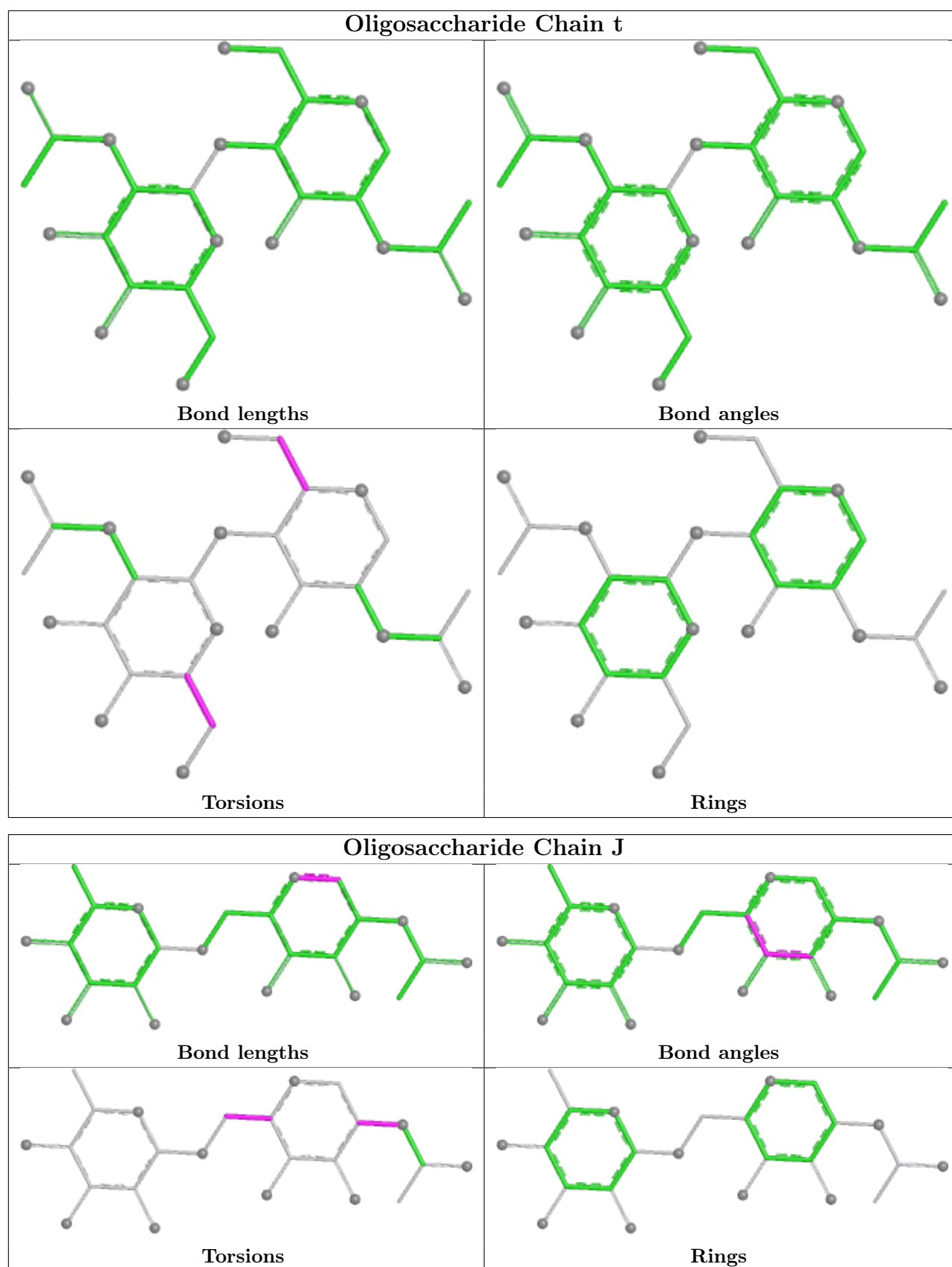


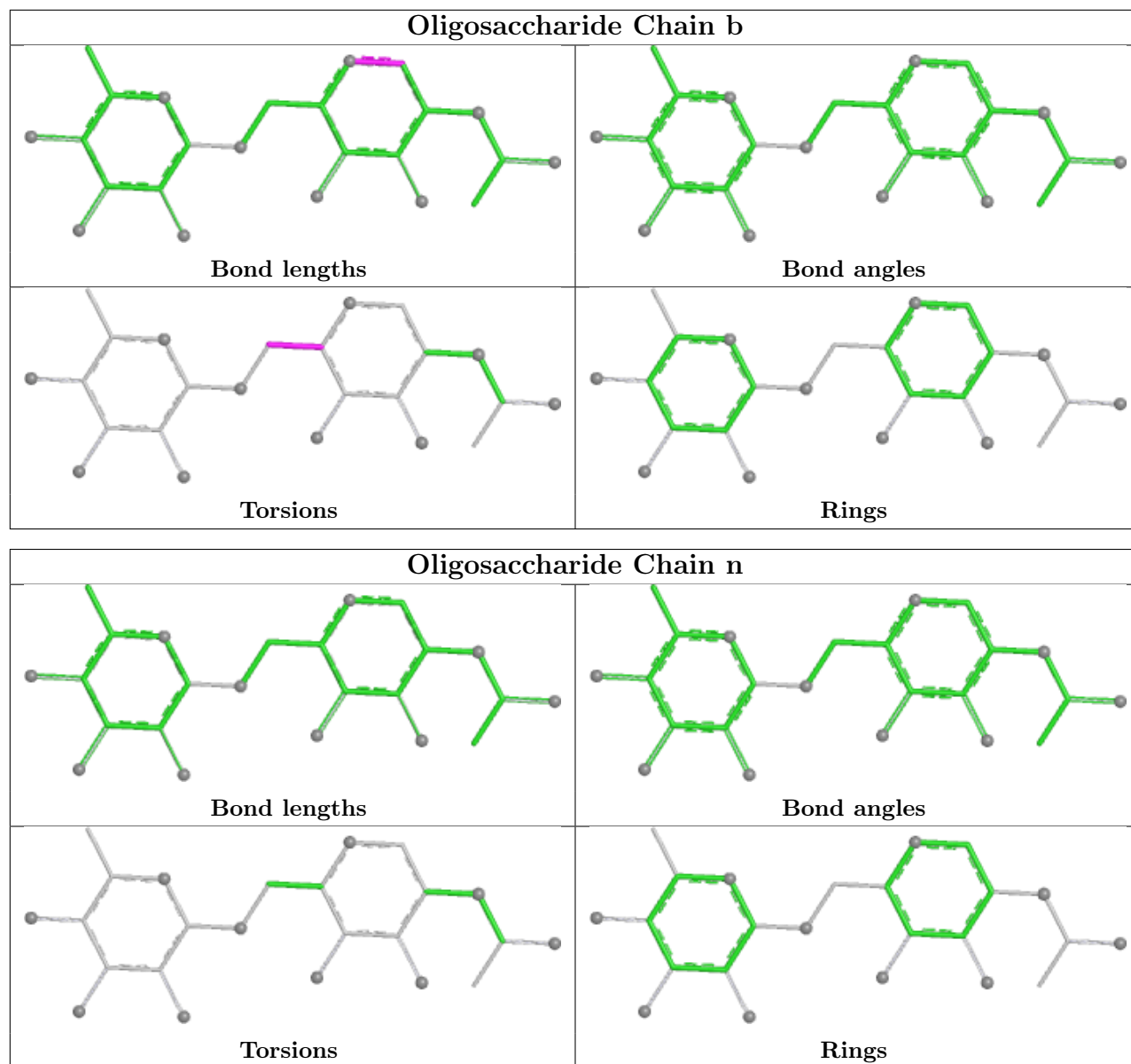


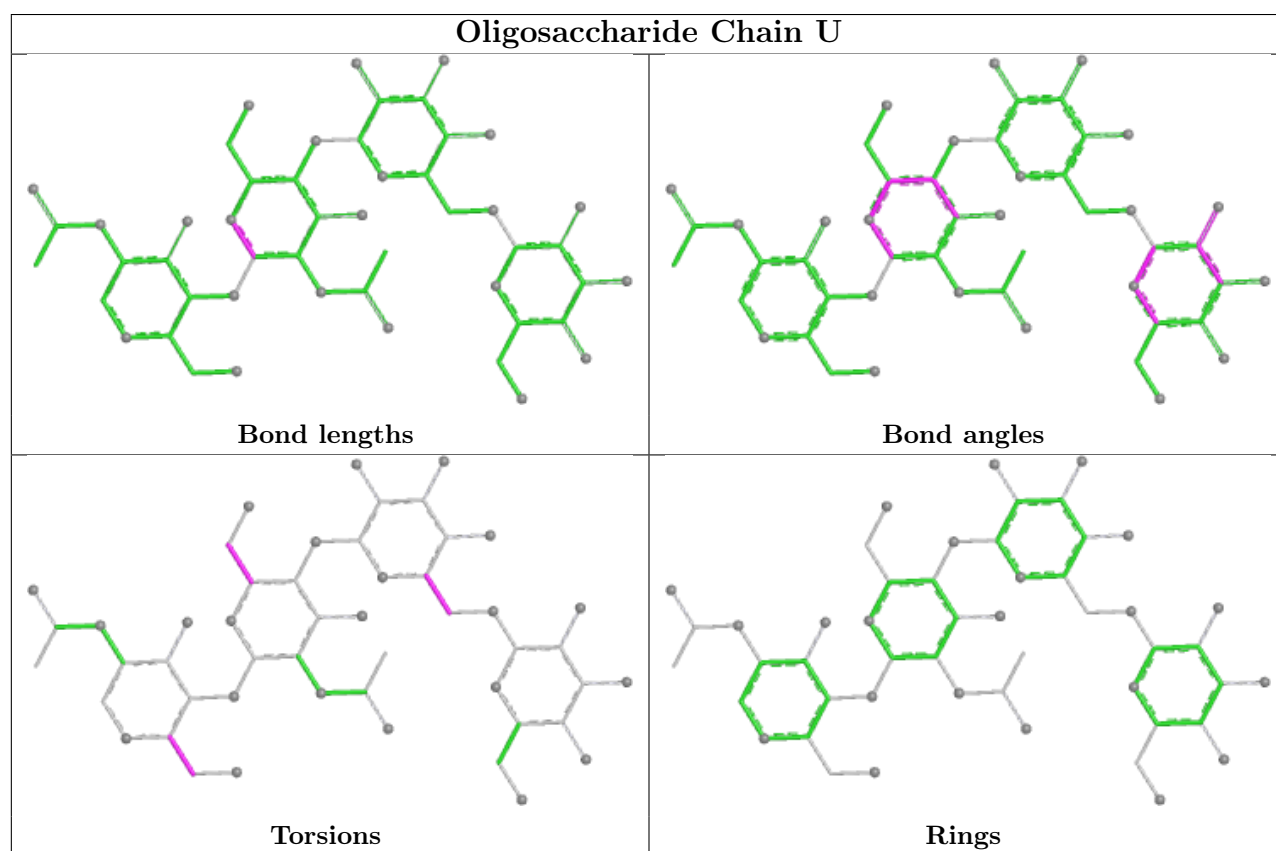
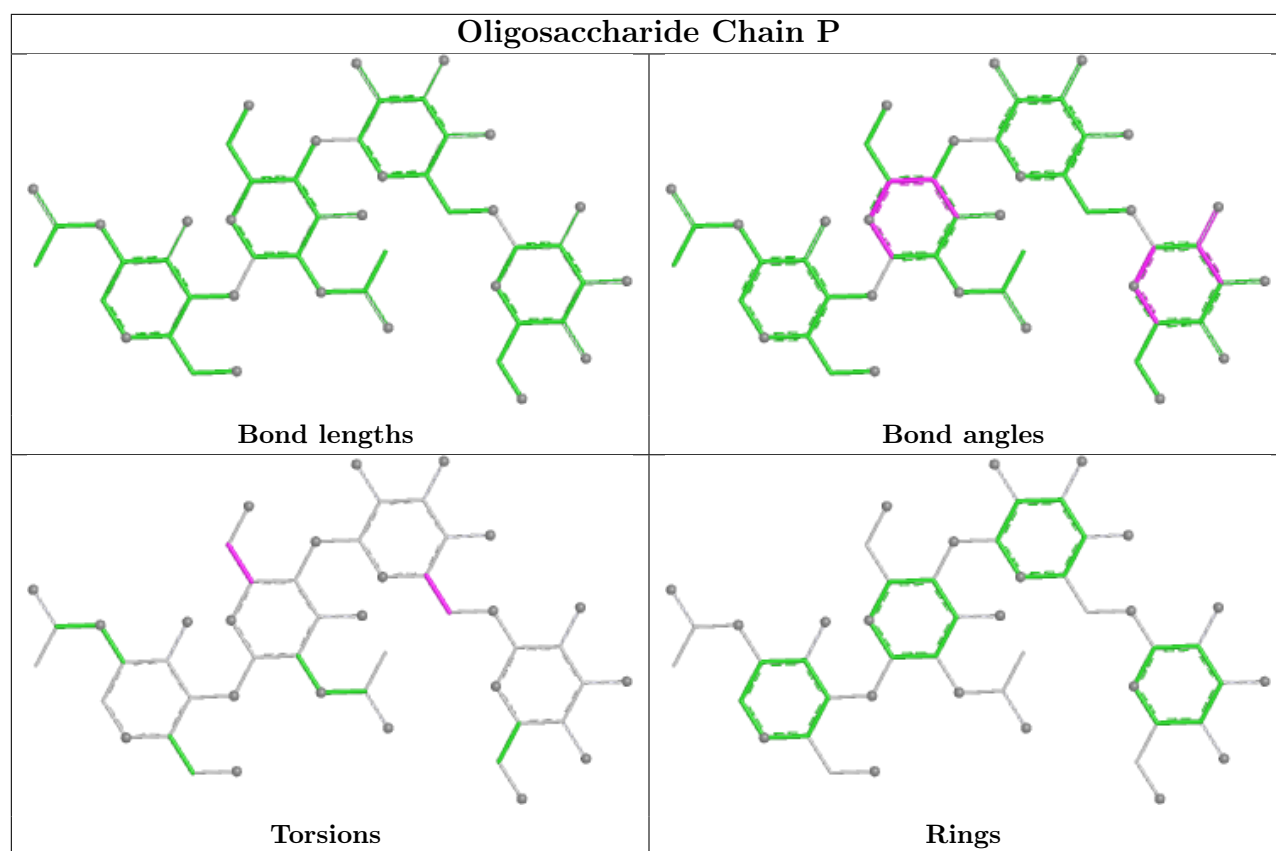


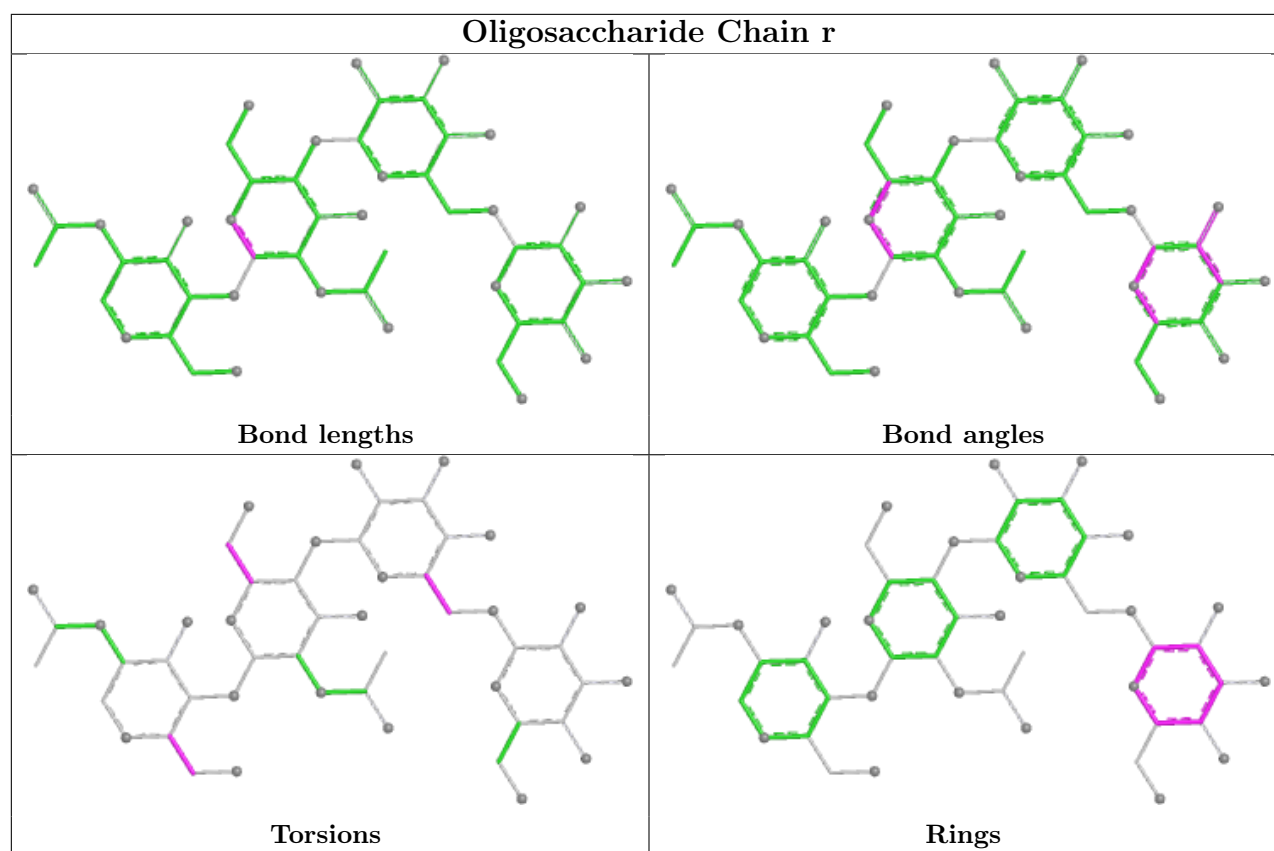












5.6 Ligand geometry [i](#)

3 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	$\# Z > 2$
8	NAG	C	1300	1	14,14,15	0.24	0	17,19,21	0.36	0
8	NAG	A	1300	1	14,14,15	0.53	0	17,19,21	0.54	0
8	NAG	B	1300	1	14,14,15	0.23	0	17,19,21	0.36	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
8	NAG	C	1300	1	-	2/6/23/26	0/1/1/1
8	NAG	A	1300	1	-	2/6/23/26	0/1/1/1
8	NAG	B	1300	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	C	1300	NAG	O5-C5-C6-O6
8	A	1300	NAG	C4-C5-C6-O6
8	A	1300	NAG	O5-C5-C6-O6
8	C	1300	NAG	C4-C5-C6-O6
8	B	1300	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

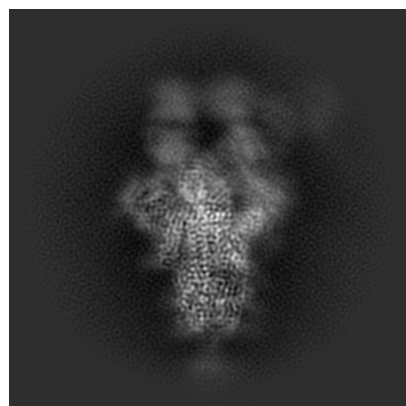
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22748. These allow visual inspection of the internal detail of the map and identification of artifacts.

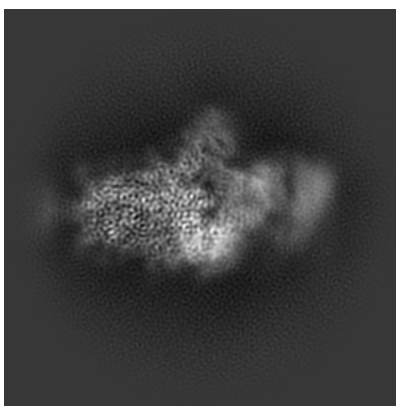
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

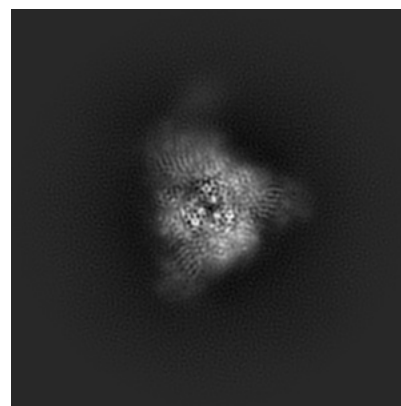
6.1.1 Primary map



X

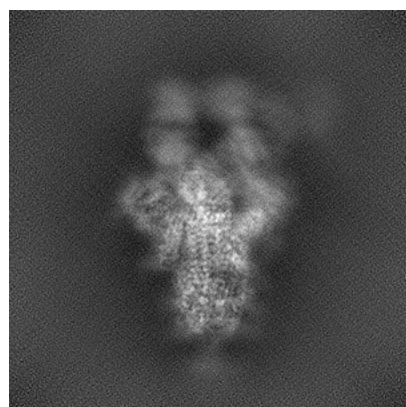


Y

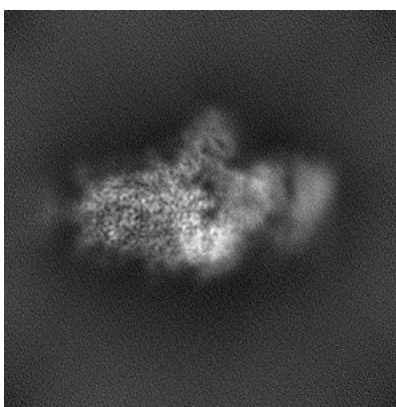


Z

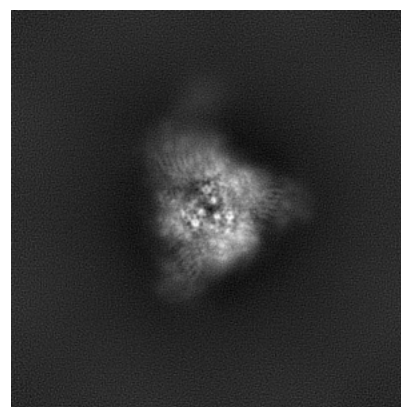
6.1.2 Raw map



X



Y

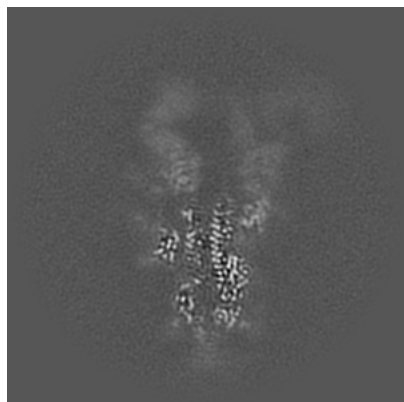


Z

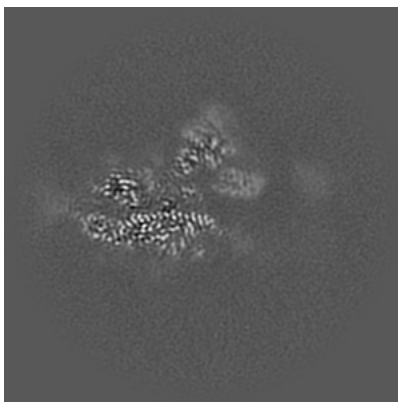
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

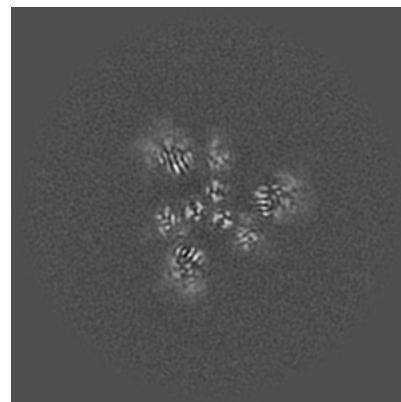
6.2.1 Primary map



X Index: 150

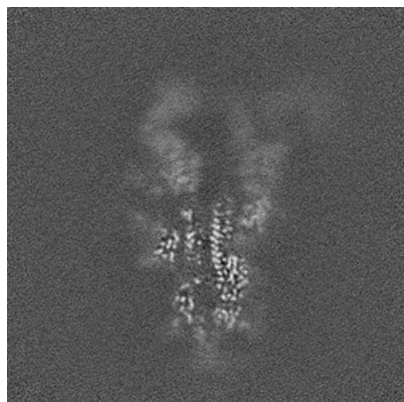


Y Index: 150

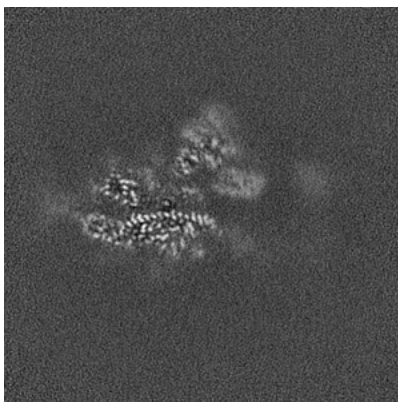


Z Index: 150

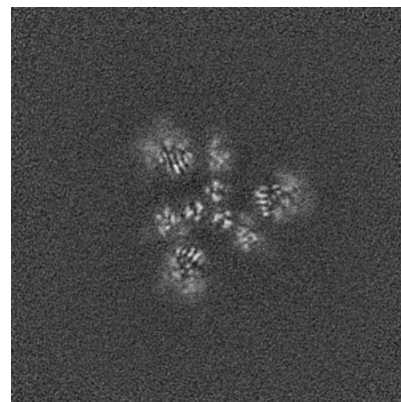
6.2.2 Raw map



X Index: 150



Y Index: 150

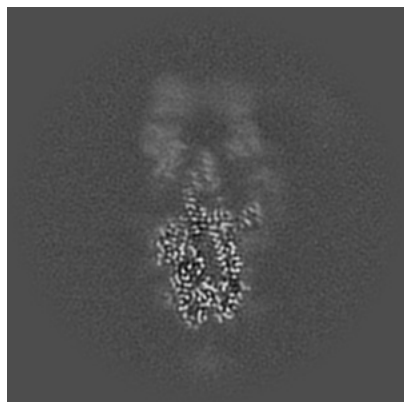


Z Index: 150

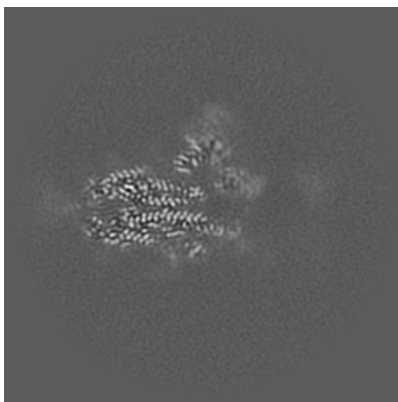
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

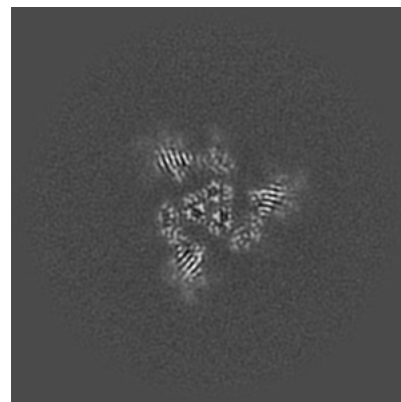
6.3.1 Primary map



X Index: 160

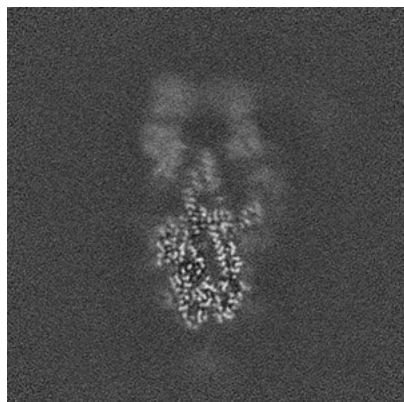


Y Index: 147

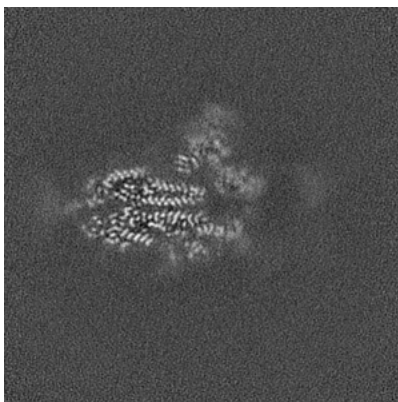


Z Index: 146

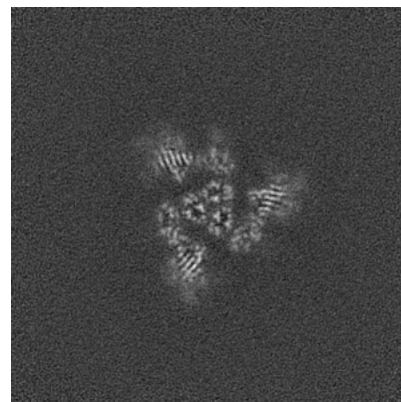
6.3.2 Raw map



X Index: 160



Y Index: 146

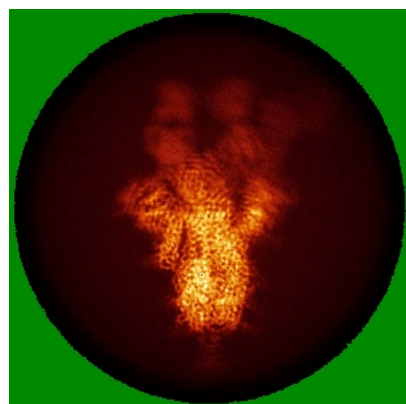


Z Index: 146

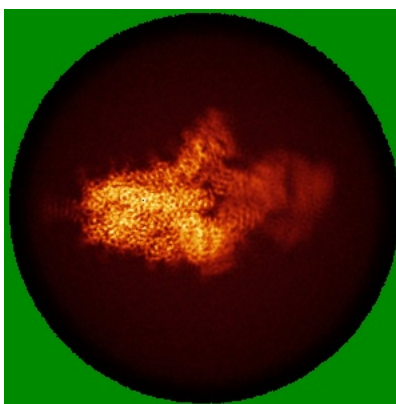
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

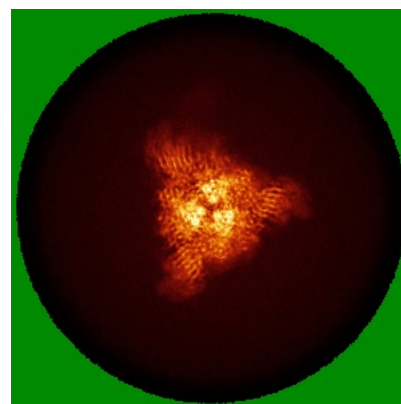
6.4.1 Primary map



X

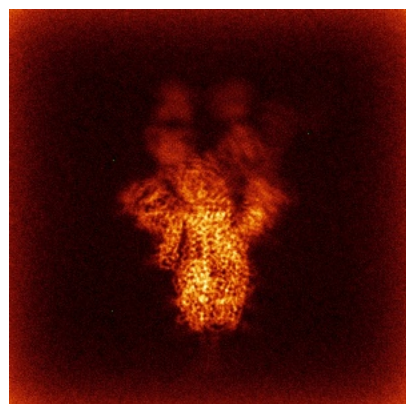


Y

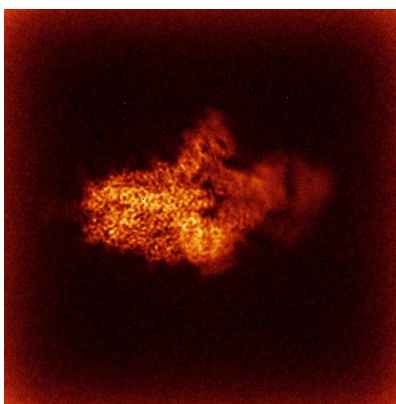


Z

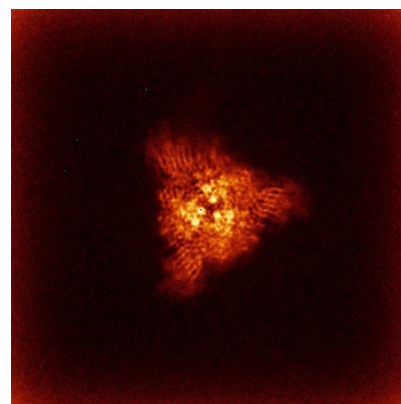
6.4.2 Raw map



X



Y

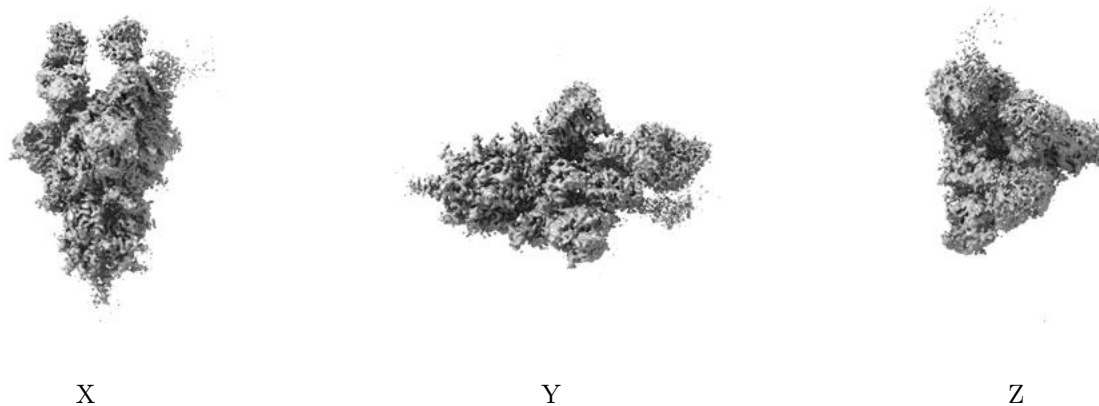


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

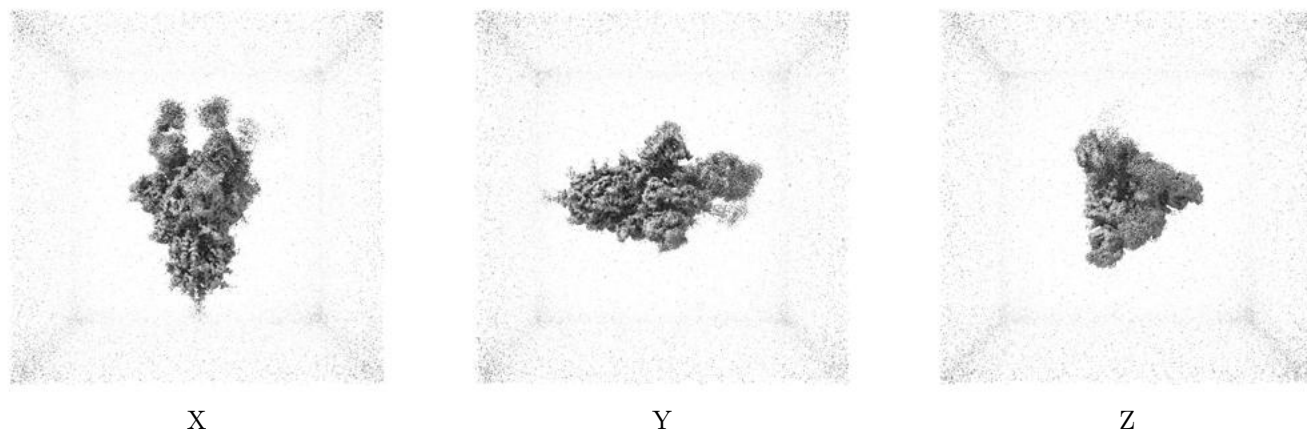
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.25. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

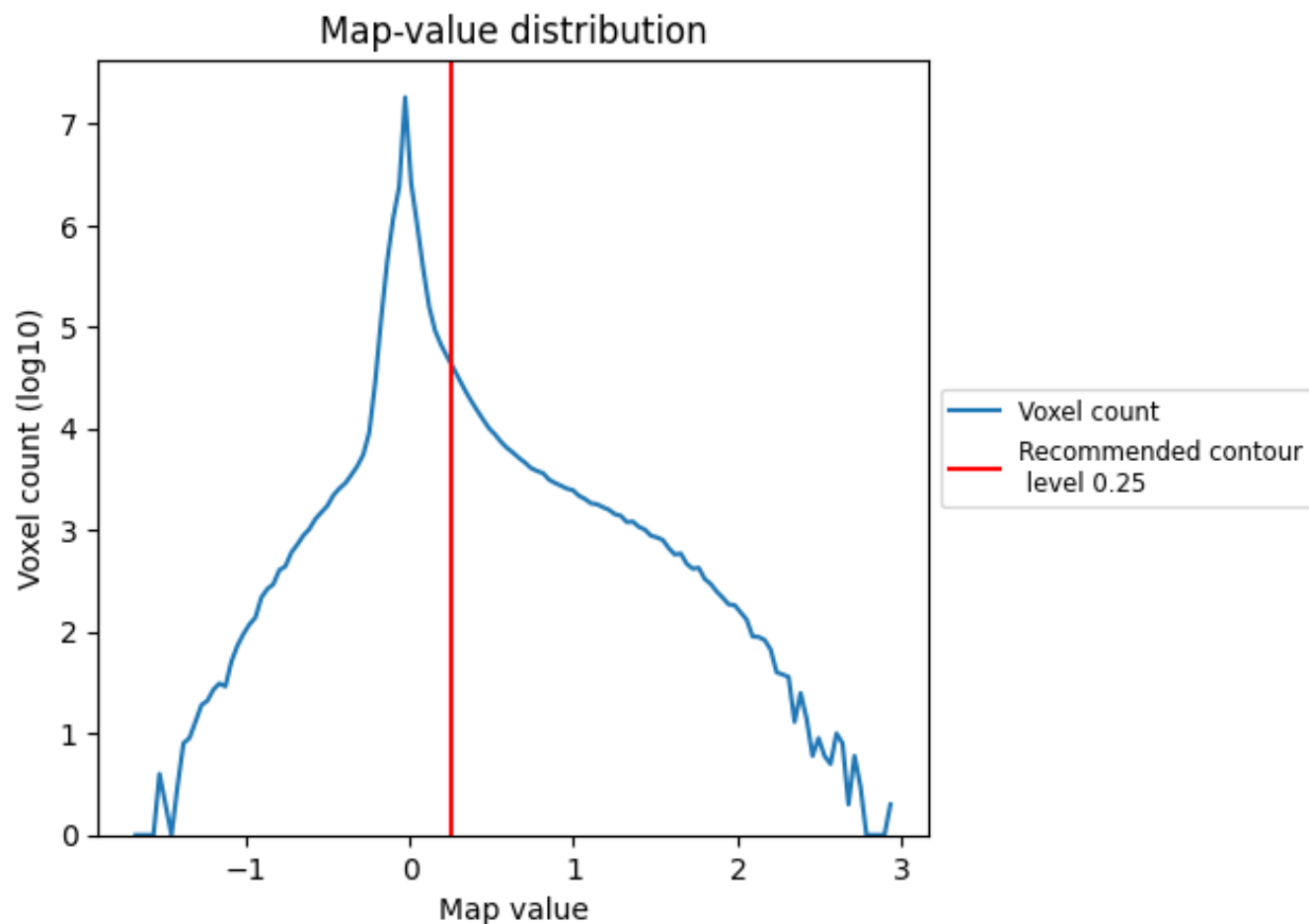
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

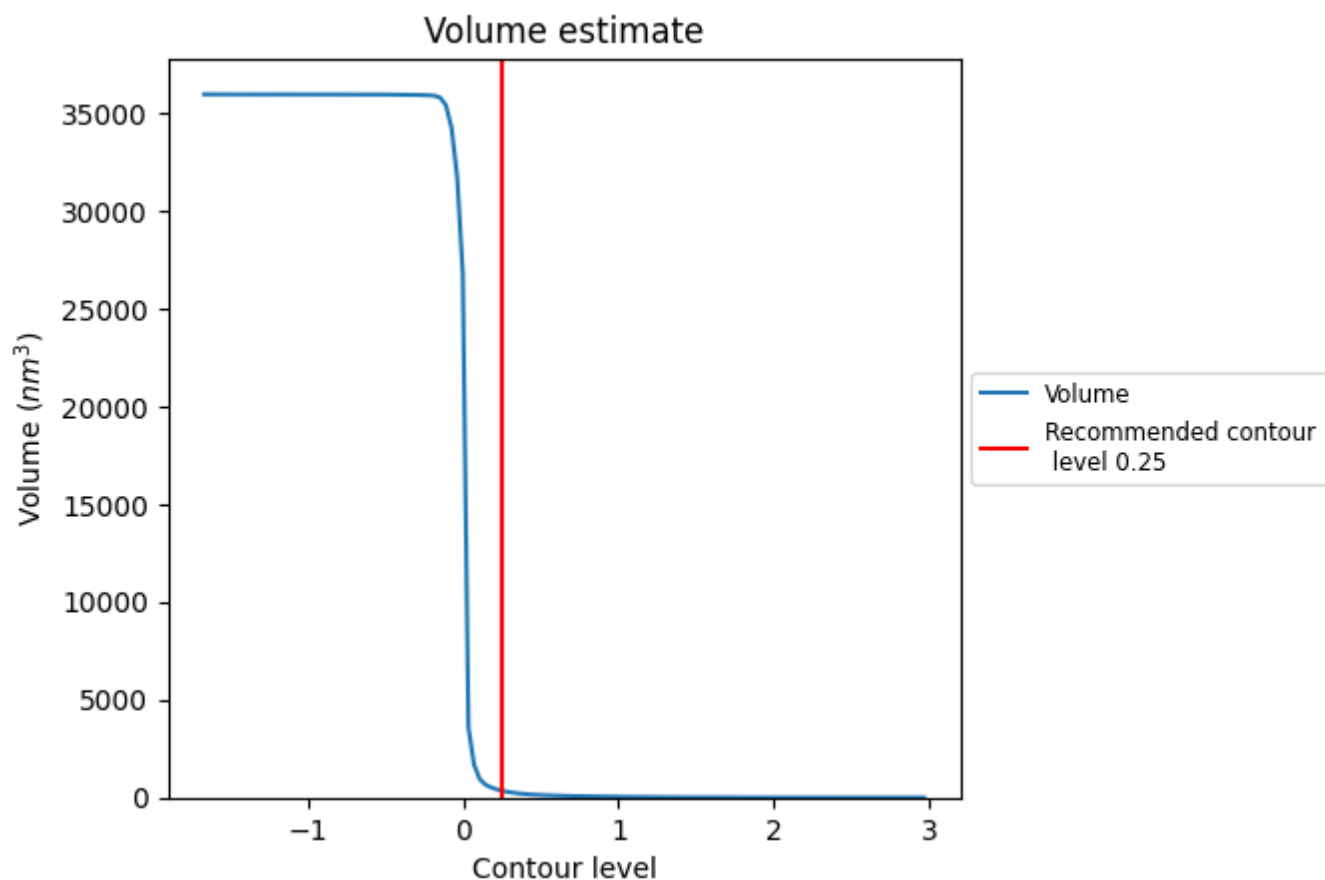
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

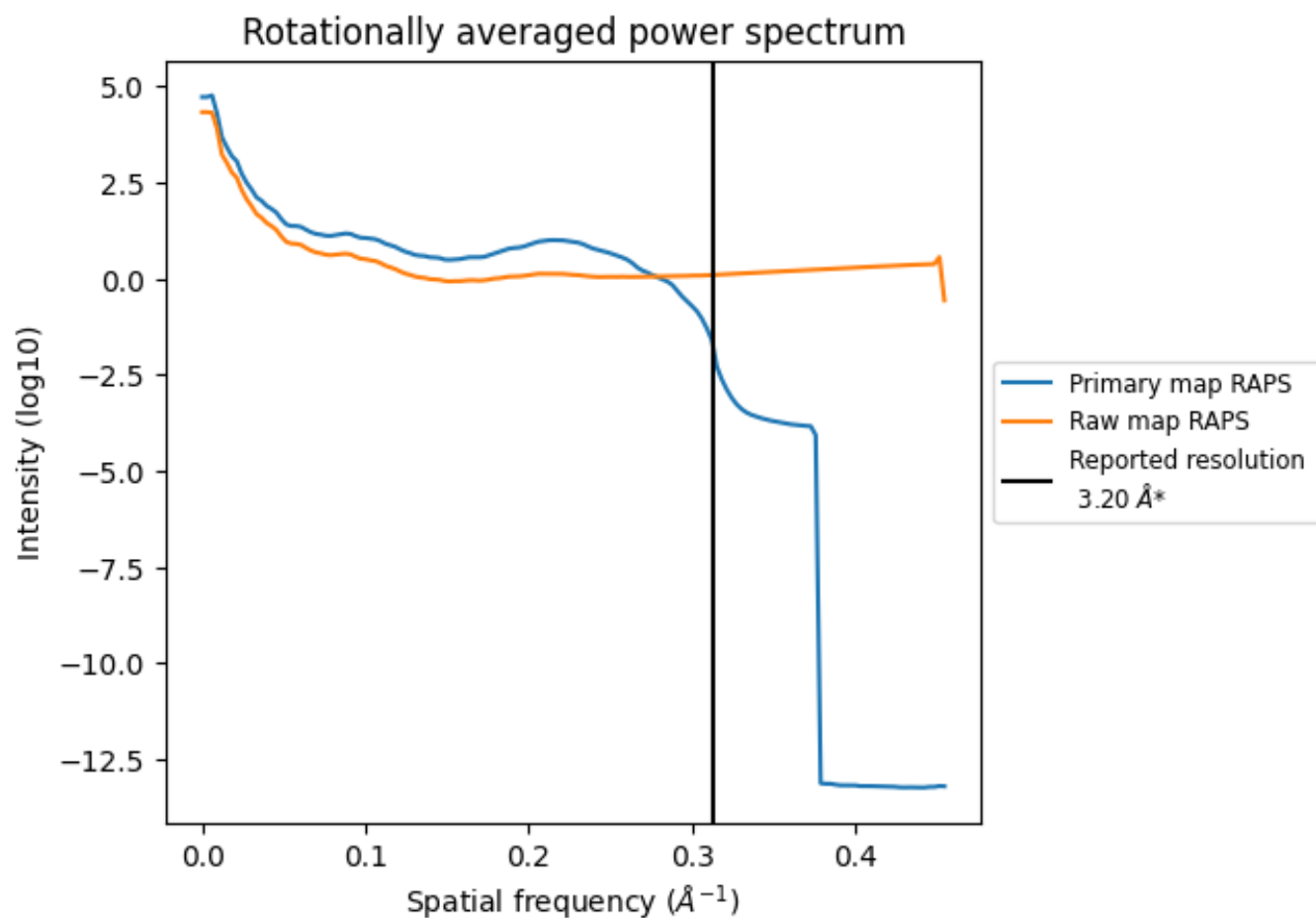
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 348 nm³; this corresponds to an approximate mass of 314 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

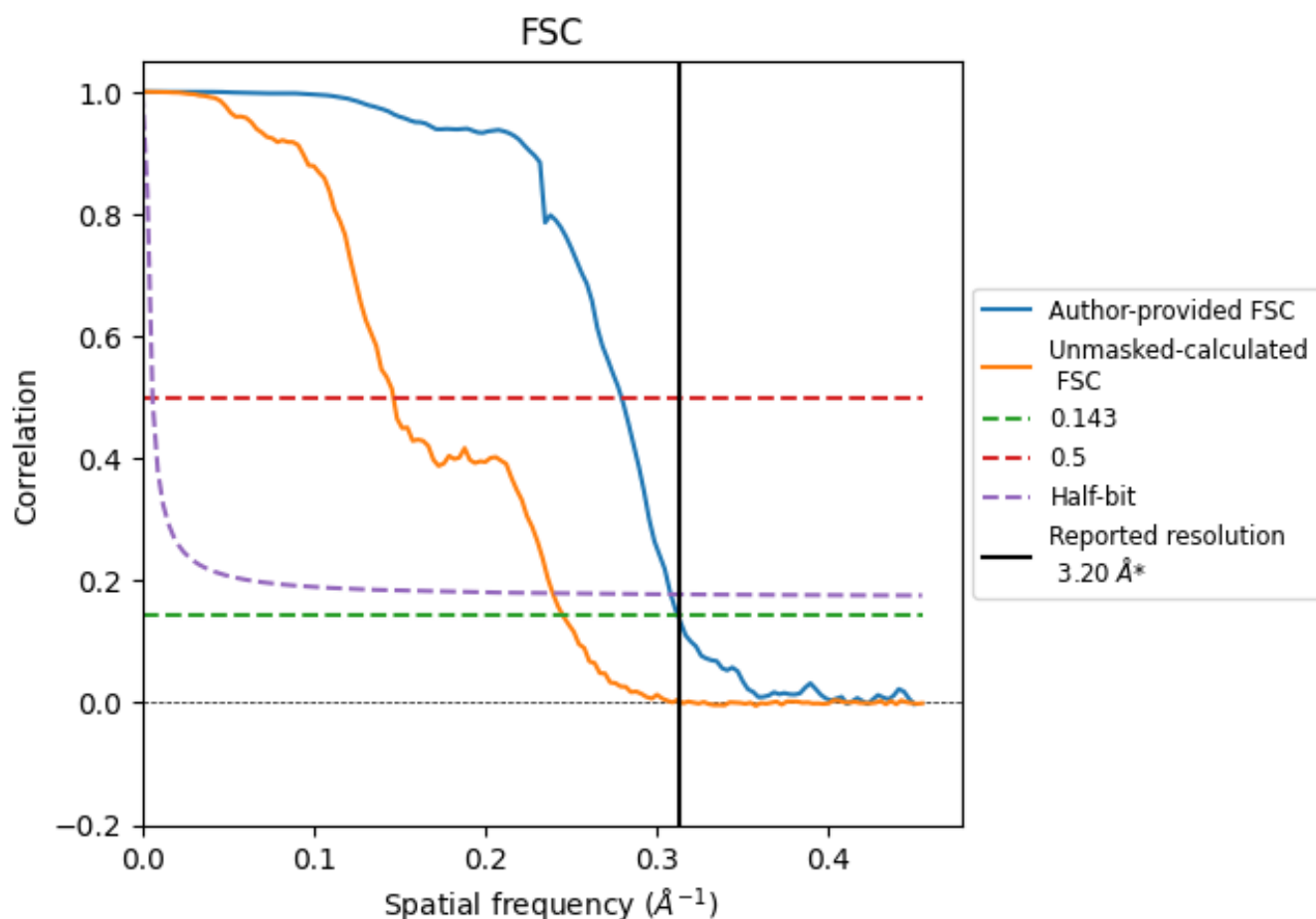


*Reported resolution corresponds to spatial frequency of 0.312 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.312 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

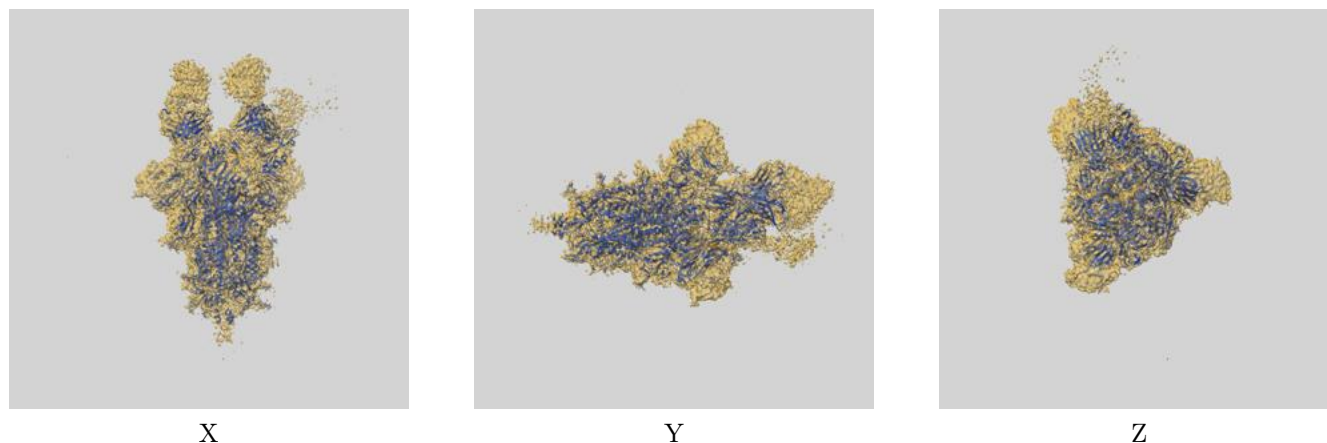
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.20	3.58	3.25
Unmasked-calculated*	4.08	6.84	4.18

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.08 differs from the reported value 3.2 by more than 10 %

9 Map-model fit [i](#)

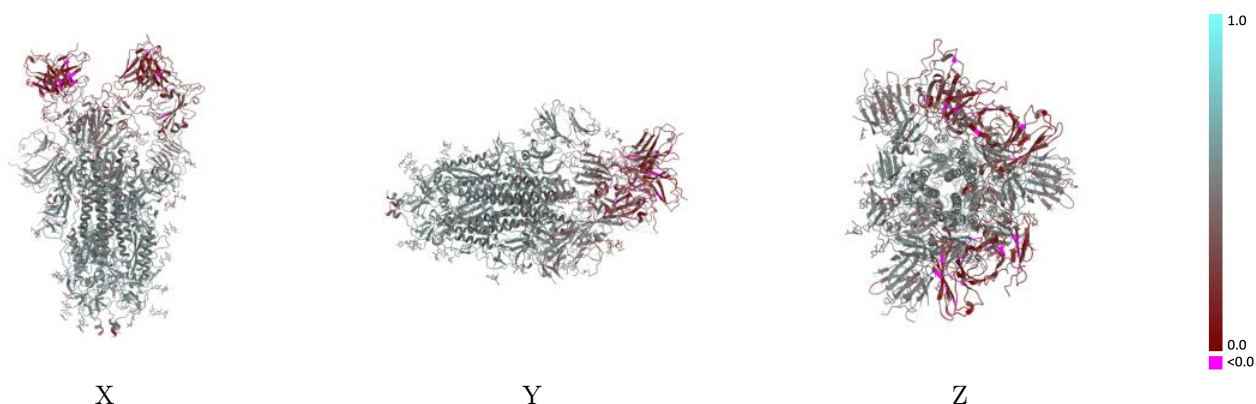
This section contains information regarding the fit between EMDB map EMD-22748 and PDB model 7K9H. Per-residue inclusion information can be found in [section 3](#) on [page 13](#).

9.1 Map-model overlay [i](#)



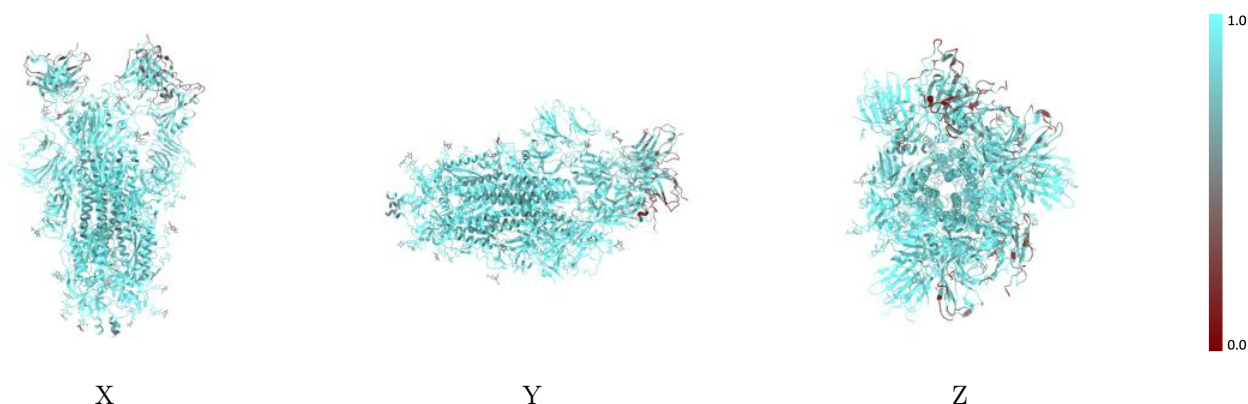
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



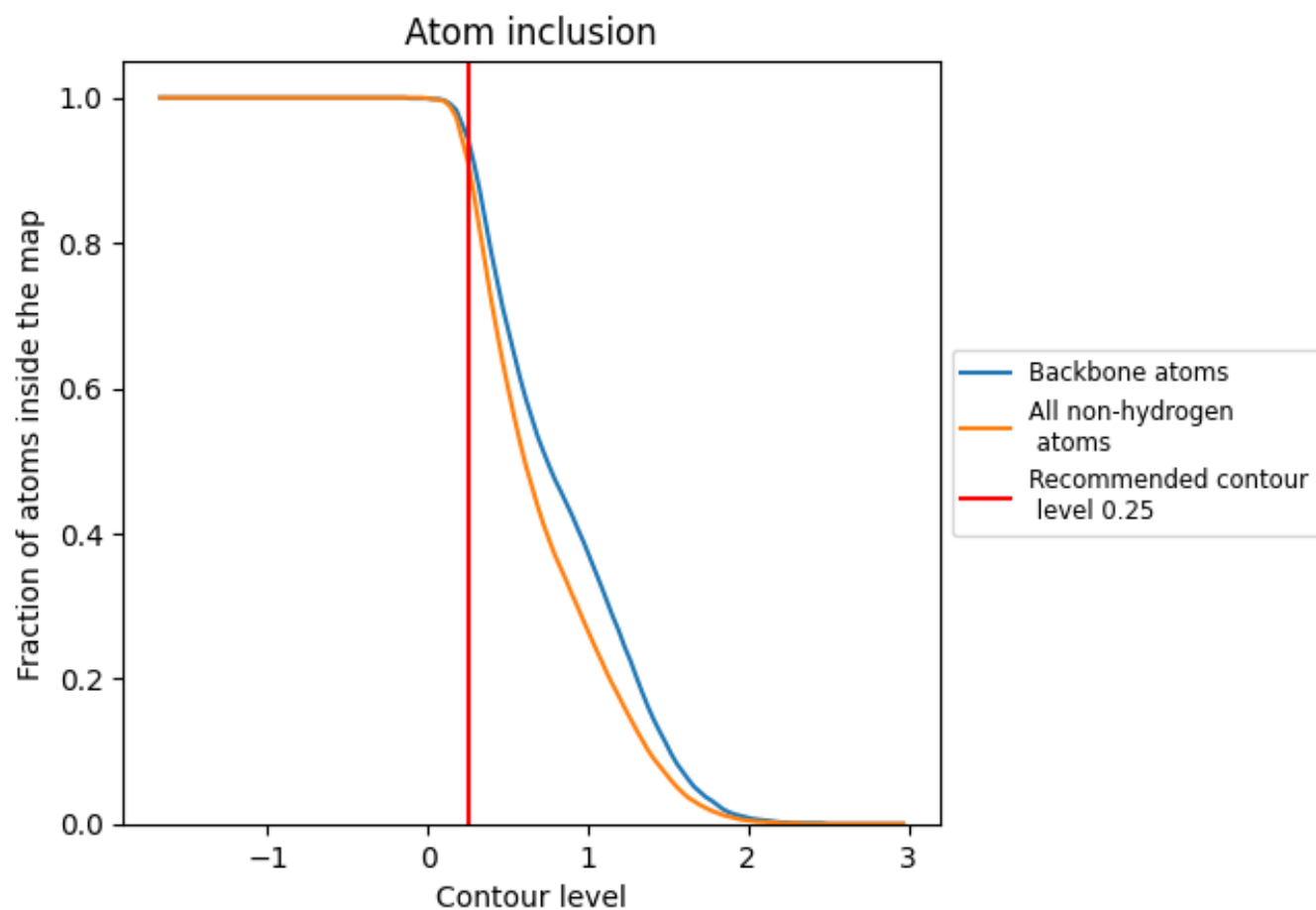
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.25).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 91% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9130	 0.4550
A	 0.9460	 0.4960
B	 0.9620	 0.4980
C	 0.9600	 0.5000
D	 0.6150	 0.3600
E	 0.6410	 0.3640
F	 0.8930	 0.3460
G	 0.9290	 0.3740
H	 0.7390	 0.2310
I	 0.7730	 0.1660
J	 0.5000	 0.3740
K	 0.8930	 0.3930
L	 0.5650	 0.2000
M	 0.7100	 0.2000
N	 0.5000	 0.4170
O	 0.8210	 0.3900
P	 0.7400	 0.4780
Q	 0.9290	 0.4610
R	 0.7500	 0.4890
S	 0.8460	 0.4360
T	 0.7690	 0.4700
U	 0.7400	 0.4600
V	 0.6920	 0.3590
W	 0.6670	 0.4130
X	 0.9290	 0.3920
Y	 0.6790	 0.3430
Z	 0.7500	 0.3560
a	 0.5900	 0.3970
b	 0.5000	 0.3960
c	 0.6430	 0.4190
d	 0.7500	 0.3770
e	 0.7950	 0.4580
f	 0.9290	 0.4890
g	 0.8570	 0.5290
h	 0.6670	 0.4120



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Chain	Atom inclusion	Q-score
i	 0.7180	 0.3550
j	 0.5130	 0.3810
k	 0.9290	 0.4010
l	 0.8210	 0.3650
m	 1.0000	 0.4280
n	 0.4580	 0.4460
o	 0.8930	 0.3540
p	 0.6430	 0.3270
q	 0.7140	 0.3800
r	 0.8200	 0.4600
s	 0.9290	 0.4260
t	 0.8570	 0.4930
u	 0.8460	 0.4750
v	 0.7180	 0.4150